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Description of the New Version 4.0 of the Tritium Model UFOTRI Including User Guide

W. Raskob
Institut für Neutronenphysik und Reaktortechnik
Projekt Kernfusion

Kernforschungszentrum Karlsruhe

KERNFORSCHUNGSZENTRUM KARLSRUHE
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Projekt Kernfusion

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of the tritium model UFOTRI
including user guide

W. Raskob *

* D.T.I. Dr. Trippe Ingenieurgesellschaft m.b.H.

Kernforschungszentrum Karlsruhe GmbH, Karlsruhe

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Abstract

In view of the future operation of fusion reactors the release of tritium may play a dominant role during normal operation as well as after accidents. Because of its physical and chemical properties which differ significantly from those of other radionuclides, the model **UFOTRI** for assessing the radiological consequences of accidental tritium releases has been developed. It describes the behaviour of tritium in the biosphere and calculates the radiological impact on individuals and the population due to the direct exposure and by the ingestion pathways. Processes such as the conversion of tritium gas into tritiated water (HTO) in the soil, re-emission after deposition and the conversion of HTO into organically bound tritium, are considered. The use of UFOTRI in its probabilistic mode shows the spectrum of the radiological impact together with the associated probability of occurrence.

A first model version was established in 1991. As the ongoing work on investigating the main processes of the tritium behaviour in the environment shows up new results, the model has been improved in several points. The following report describes the changes incorporated into the model since 1991. Additionally provides the up-dated user guide for handling the revised UFOTRI version which will be distributed to interested organizations.

Programm- und Eingabebeschreibung der neuen Version 4.0 des Tritiummodells UFOTRI

Zusammenfassung

Im Hinblick auf den Betrieb von Fusionsreaktoren spielt die Freisetzung des Radionuklids Tritium sowohl während des Normalbetriebes als auch im Anschluß an einen Unfall eine bedeutende Rolle. Wegen seiner physikalischen und chemischen Eigenschaften, die deutlich von denen anderer Radionuklide abweichen, wurde das Computermodell **UFOTRI** erstellt, das nach einer unfallbedingten Freisetzung das Verhalten von Tritium in der Biosphäre beschreibt und die Belastung des Menschen über direkte Exposition und den Nahrungsmittelpfad berechnen kann. Hierbei müssen Prozesse wie die Umwandlung von HT in HTO im Boden, die Reemission des HTO nach der Ablagerung und die Umwandlung von HTO in organisch gebundenes Tritium mit berücksichtigt werden. Der Einsatz von UFOTRI zur probabilistischen Dosisabschätzung weist nicht nur die reinen Dosiswerte aus, sondern stellt gleichfalls die Eintrittshäufigkeit dieser Ereignisse dar.

Eine erste Version des Rechenprogramms wurde 1991 fertiggestellt. Nach der Auswertung neuer experimenteller Arbeiten ergab sich die Notwendigkeit UFOTRI in einigen Bereichen zu erweitern und zu ertüchtigen. Der jetzige Bericht beschreibt die Änderungen gegenüber 1991. Vervollständigt wird er durch eine Eingabebeschreibung, die interessierten Benutzern die Arbeit mit dem Rechenprogramm erleichtern soll.

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4. Introduction

The model UFOTRI for assessing the radiological consequences of accidental tritium releases describes the behaviour of tritium in the biosphere and calculates the radiological impact on individuals and the population due to inhalation, skin absorption and incorporation of contaminated foodstuffs. To estimate the spectrum of consequences after accidental releases of tritium from nuclear installations, processes such as dispersion, deposition, reemission, conversion of tritium gas (HT) into tritiated vapour (HTO) and conversion of HTO into organically bound tritium (OBT), had to be considered time dependent. To that purpose, an atmospheric dispersion module has been developed which allows for reemission after HT/HTO deposition and which considers all relevant transfer processes in the environment (soil, plant and animal) up to approximately 100 hours after the release event (during which the atmospheric transport plays the dominant role). It was coupled to a first order compartment module, which describes dynamically the longer-term behaviour of the two different chemical forms of tritium in the food chains.

The UFOTRI model was established in a first version in mid 1991. The physical and mathematical basis of this code version is described in detail in /24/. Since 1991 the model has been further developed in several parts, especially in the

- plant / atmosphere exchange model,
- soil / atmosphere exchange model,
- plant model,
- photosynthesis model (OBT-formation).

This report summarizes the most important features of the UFOTRI program but concentrates mainly on the model extensions. The report follows the structure of UFOTRI which is mainly divided into a dynamic part followed by a compartment module calculating the longer term behaviour of tritium in the foodchains. In the first part of the report the mathematical and physical models are described for the time shortly after the accident whereas the second part describes the derivation of the transfer rates included in the compartment module. Additionally, the up-dated user guide completes this report.

5. Model description

5.1 Atmospheric dispersion processes

This part is mainly identical to the initial model, therefore, only a broad model description is given. The present version is based on the Gaussian trajectory model MUSEMET /36/ which was slightly modified for describing the behaviour of tritium in the environment in both chemical forms, gaseous tritium and tritiated water vapour. The importance of the reemission process necessitates two level modelling of the atmospheric dispersion. Primarily, MUSEMET calculates the dispersion after a single release event and the subsequent deposition on soil and plants. In a second step, the reemission of tritium

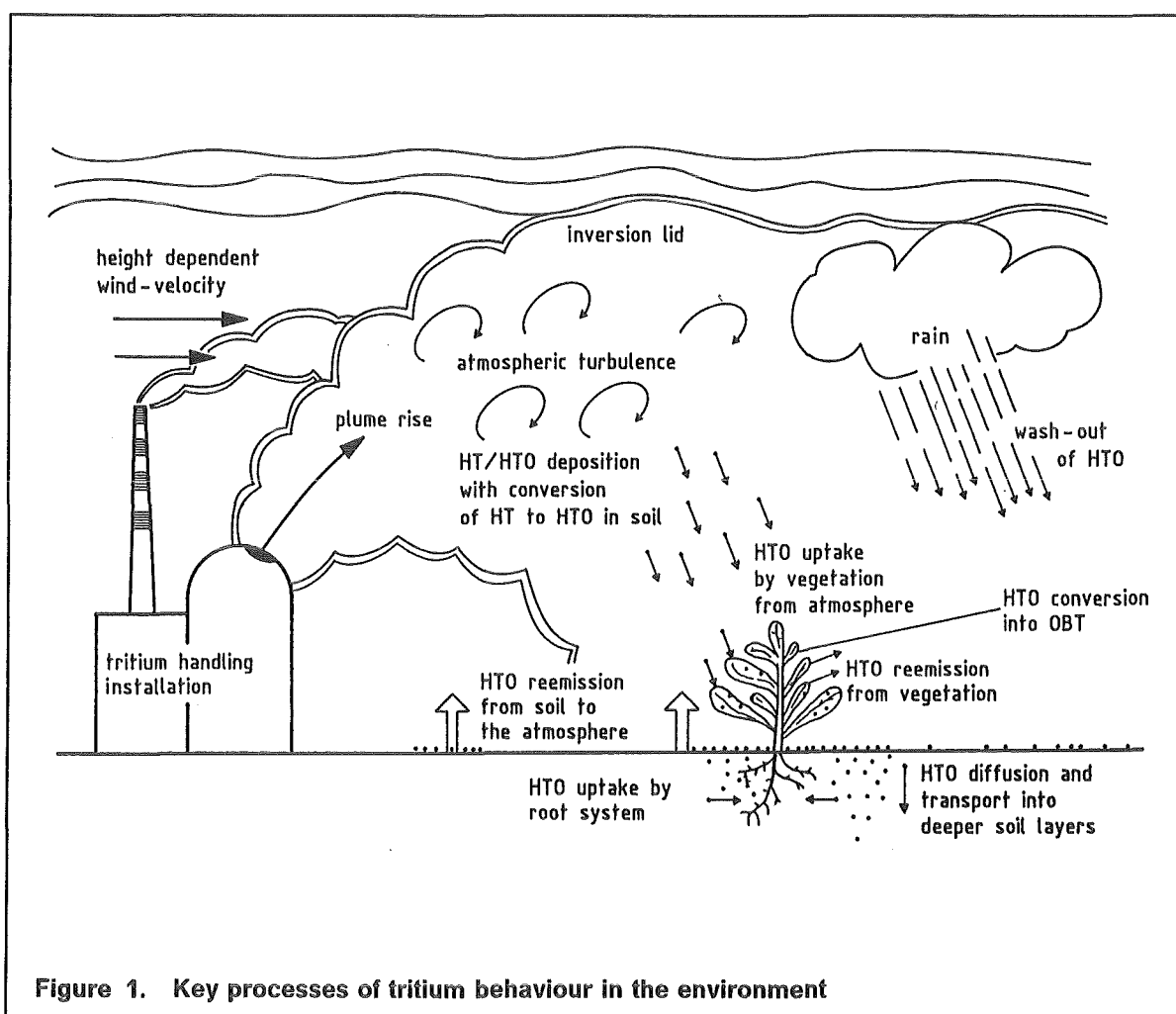


Figure 1. Key processes of tritium behaviour in the environment

after deposition from soil (evaporation) and plants (transpiration) is taken into account by an area source model specially developed for that purpose and combined with the original model. The exact solution of the Gaussian algorithm of such an area source model - a double integral - would require a large amount of computing time. Therefore a

simplified assumption which replaces the area source by a single source point in the centre of the area, with a given initial widening of the plume, is used in UFOTRI. /37/.

All processes, which may modify the total balance of the available HT or HTO such as the conversion of tritium gas into tritiated water (HT into HTO), the transport of tritium into deeper soil layers, the uptake of tritium by the plant root system, and the conversion of HTO into OBT are taken into account in the atmospheric dispersion module (Fig. 1), together with the foodchain pathways such as the production of milk, milk products and beef.

5.2 Plant/atmosphere exchange processes

The exchange reaction of the plant with the atmospheric tritium takes place via the water circulation in the leaves. This process of direct uptake is negligible in case of an HT release /33/. The mechanisms of the plant/atmosphere exchange are described according to the model of Belot /2/. There, the temperature, the anorganic content of plant matter and the transfer resistances (aerodynamic r_{av} , boundary layer r_{bv} and stomata r_{st} resistance) determine the uptake of tritium in the vegetation as well as the loss of tritium from the vegetation. With the assumption of stationarity within one time step the following equation may be derived:

$$C = \chi \frac{\alpha}{\rho} (1 - e^{-lt}) \quad (1)$$

with

$$l = \frac{\rho}{\alpha \mu r_g} \quad (2)$$

where

- l = the time constant for reaching equilibrium in s^{-1} ,
- μ = water content per unit area of leaf in $g \text{ cm}^{-2}$
- χ = concentration of tritium in air in $Bq \text{ ml}^{-1}$
- C = tritium concentration in tissue water in $Bq \text{ g}^{-1}$
- r_g = total resistance in $s \text{ cm}^{-1}$
- t = time in s
- ρ = density of water vapour in saturated air in $g \text{ ml}^{-1}$ and
- α = H/T isotope ratio in liquid and air, assumed to be 1.1.

From this equation, the contamination of the plant can be determined directly if the ground level air concentration is known. Any loss of concentration from the plant is also determined by the time constant l :

$$\delta C = C_0 e^{-lt} \quad (3)$$

The dominating factor controlling the tritium flux is the total transfer resistance r_g .

$$r_g = r_{st} + r_{av} + r_{bv} \quad (4)$$

The stomata resistance will be modified to a canopy resistance r_c , valid for a whole vegetation population (see above).

The aerodynamic resistance r_{av} characterizes the transfer from the free atmosphere to the surroundings of the leaf, whereas the boundary layer resistance r_{bv} describes the mass transfer through the quasi laminar air layer directly connected to the surface /19/, /4/.

$$r_{av} = \frac{u(z)}{u_x^2} \quad (5)$$

$$r_{bv} = \frac{1}{u_x} B^{-1} \quad (6)$$

where

- $u(z)$ = wind speed in m/s in a given height (10m)
- u_x = friction velocity in m/s
- B = Stanton number

Since r_{av} and r_{bv} depend on the atmospheric stability and the surface properties, the logarithmic wind profile together with the Dyer-Businger equations are used in calculating u_x . /4/.

The stomata resistance r_{st} describes the transfer through the leaf epidermis into the plant. In the present version of UFOTRI two possibilities of calculating the stomata resistance are offered. The simple one uses only the parameters water content in the soil and solar insolation, which is divided into a daylight and night-time period. The extended plant model for calculating the stomata resistance r_{st} considers the type of plant, the temperature, the photosynthetically active radiation, the humidity of the air and the water content in the soil /1/, /10/ and /17/.

$$r_{st} = r_{st,m} \left[1 + \left(\frac{c}{I_p} \right) \right] \frac{1}{f_i f_w f_t} \quad (7)$$

with f_i , the weighting function for humidity

$$f_i = 1 - b_v \Delta e$$

with f_t , the weighting function for temperature

$$f_t = \left[\frac{(T - T_e)}{(T_0 - T_e)} \right] \left[\frac{(T_h - T)}{(T_h - T_0)} \right]^{B_t} \quad (8)$$

with

$$B_t = \frac{(T_h - T_0)}{(T_0 - T_e)} \quad (9)$$

with f_w , the weighting function for soil water content which follows roughly a step function

where

- $r_{st,m}$ = minimum stomata resistance in s/m,
- I_p = net radiation balance in W/m^2
- Δe = vapour pressure deficit in hPa
- b_v = slope of the linear reduction function with increasing humidity deficit for a given plant species in 1/hPa
- c = constant equal to the photosynthetically active radiation (PAR) (here = half of the positive net radiation balance) flux density at twice the minimum stomata resistance in W/m^2
- T = actual temperature
- T_0 = optimal temperature for photosynthesis (plant species dependent),
- T_h = upper limit of the temperature for photosynthesis (plant dependent)
- T_e = lower limit of the temperature for photosynthesis (plant dependent)

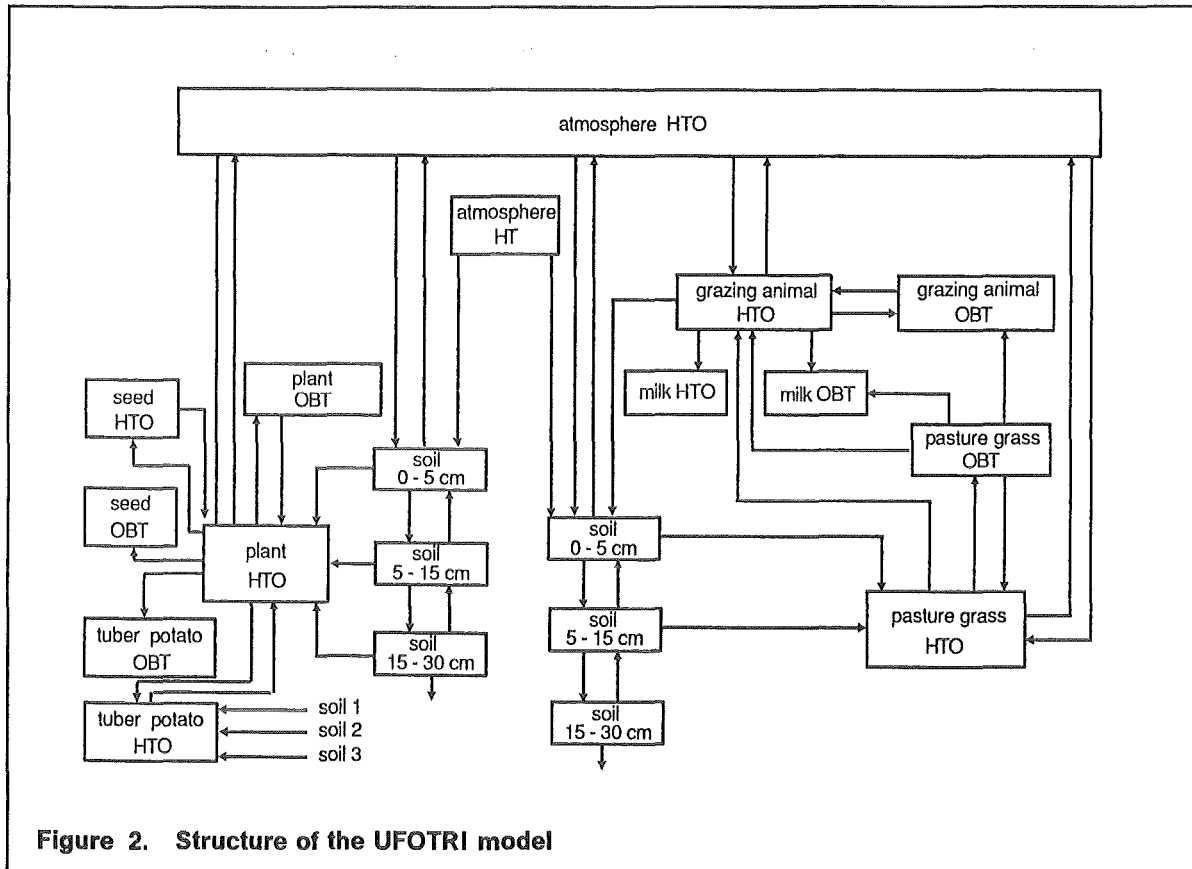
For all of these variables, default values are included in the code, which may be easily changed by the user.

At night, the plant stomata, in which over 90% of the water vapour exchange takes place, are usually closed, and exchange takes place only via the plant epidermis whose resistance is higher by at least a factor of 10 to 15 than the stomata resistance /28/.

In case of precipitation, it is assumed that the stomata resistance goes towards a very small value and only the atmospheric resistance is relevant. At night, when the stomata are closed, the leaf resistance (now, the epidermal resistance) remains constant also in case of rain.

Because vegetation mainly appears in the form of plant populations (fields, forests, etc.), an effective stomata resistance (now canopy resistance r_c) has to be calculated. This is done by dividing the stomata resistance of a single plant by the leaf area index L which describes the area of all leaves of the vegetation normalized to one square meter.

$$r_c = \frac{1}{L} r_{st} \quad (10)$$



UFOTRI considers four different plant species, namely nutrient plants (leafy vegetables, potatoes and wheat) and pasture grass. Because of the plant specific parameters describing the exchange processes plant/environment, the model has to account for four different areas, three covered with nutrient plants and one for pasture grass. Due to missing land-use data, at present it is not possible in the model to consider a site specific distribution of the four areas. So it is assumed that each grid point which is representative of a certain grid area contains pasture grass as well as cultivation fields for nutrient plants with percentage contributions selected by the user.

5.3 Soil/atmosphere exchange processes and transport in soil

For calculating the loss of tritium from soil, the evapotranspiration rate of water - which contains a specific tritium concentration - has been used in UFOTRI. The process of water loss from the top layer by evapotranspiration is subdivided into two separate processes, i.e. evaporation from soil on the one hand and transpiration of plants on the other hand. The reemission rate of HTO is assessed on the basis of the soil evaporation, and the plant transpiration determines the amount of water which must be transported from the root system to the plant in order to balance the loss of water. Together with the water, a given amount of tritium is taken up by the plant root system.

As described in the previous chapter the reemission of HTO from the plant is modelled by using Belot's model. This approach is a mixture of diffusion loss and loss of tritium via the water loss from transpiration of the plant. Having this in mind it is obvious, that the transpiration rate of the plant is only valid for the processes mentioned above, namely water loss and root uptake.

5.3.1 Evapotranspiration from plant and soil (water)

In the present version of UFOTRI two possibilities of calculating the evapotranspiration flux are offered. One approximation is using Penman's empirical equation (potential evapotranspiration) /23/, which combines the radiation balance and the wind effects. Introducing a reduction factor one may estimate therefrom the actual evapotranspiration rate. In UFOTRI the wind term of Penman's approach is neglected, i.e. this formula can be applied if no input data about humidity are available. The favoured (recommended) approach is using Monteith's bulk resistance formula for the actual evapotranspiration rate /4/:

$$\lambda E_a = \frac{\delta R_{n0} + \rho c_p (e_s - e_a)/r_{AV}}{\delta + \gamma (1 + r_x/r_{AV})} \quad (11)$$

where

- λ = the latent heat of evaporation in $J \text{ kg}^{-1}$,
- E_a = the actual evapotranspiration in $kg \text{ m}^{-2} \text{ s}^{-1}$,
- R_{n0} = the radiation balance in $W \text{ m}^{-2}$,
- e_a ($e_{a,s}$) = the actual (saturation) vapour pressure of air in $N \text{ m}^{-2}$,
- δ = the gradient of the vapour pressure curve at ambient temperature in $J \text{ m}^{-3} \text{ K}^{-1}$,
- γ = the psychrometer constant in $J \text{ m}^{-3} \text{ K}^{-1}$,
- r_{AV} = the atmospheric resistance = $r_{av} + r_{bv}$
- r_x = the surface resistance.

Since it is necessary to decide between transpiration of plants and evaporation of soil, the formula is used twice. The incoming radiation flux is divided in two parts, one reaches the ground and the other one is absorbed by the leaves. Consequently, the surface resistance is the soil surface resistance and the canopy resistance, respectively. The radiation flux is subdivided according to /27/ into the following:

$$R_{a,l} = R_{n0} \times (1 - e^{-0.388L}), \text{ and}$$

$$R_{a,s} = R_{n0} \times e^{-0.388L},$$

where

- $R_{a,l}$ = radiation flux absorbed by the leaves
- $R_{a,s}$ = radiation flux modified by shading of leaves reaching the soil surface
- L = leaf area index in m^2/m^2 .

The unknown variables are the resistances of soil, plants and atmosphere. The determination of the plant and atmospheric resistance has been described in the previous chapter. In the following chapter, a method for calculating the soil resistance will be presented.

5.3.2 Dry deposition of tritium to soil (including derivation of soil resistance)

The deposition process of HT and HTO to the soil is expressed in the form of a deposition velocity. The HT deposition rate depends on the type of soil and on the soil moisture. The formalism of a time dependent HT deposition velocity was adopted from /9/.

$$v_{d,HT} = \frac{D_{eff}}{r_{ref}} \quad (12)$$

with

$$D_{eff} = 0.7 \times D_0 \times \left(\frac{T_a}{273} \right)^{1.75} \times \frac{\Phi}{tort} \quad (13)$$

where

- D_{eff} = effective diffusion coefficient in m^2/s ,
- D_0 = diffusion coefficient of HT in air ($0.634E-4$) in m^2/s ,
- r_{ref} = reference depth in m (0.023 m),
- T_a = actual temperature in Kelvin,
- Φ = maximum water content in the first soil layer minus the actual water content in the first soil layer (fraction of total soil volume)
- $tort$ = tortuosity factor of soil (1.5).

Once deposited, HT is transformed into HTO very quickly as a result of microorganism activity. Only the transformed part of HT remains in the soil. In winter the deposition rate is reduced to take into account the smaller number of active microorganisms.

The dry deposition rate of HTO to soil may be calculated in two different ways. Firstly, it is assumed that it remains constant throughout the year; secondly, it depends on the status of soil and atmospheric turbulence. Then it will be expressed as the inverse of the atmospheric- and soil- exchange resistances.

$$v_{d,HTO} = \frac{1}{r_{av} + r_{bv} + r_{soil}} \quad (14)$$

where

- r_{soil} = resistance of soil in s/m

If the soil surface is wet, the soil resistance will go towards a minimum value; in all other cases the soil resistance has a fixed value. The resistances atmosphere/HTO-plant and atmosphere/HTO-soil act in parallel.

UFOTRI offers two possibilities for the selection of the soil resistance. Firstly, it is possible to use a fixed resistance value predefined by the user (default is 150 s/m) which will be modified only in case of rainfall and dew formation. Secondly, the soil resistance may be calculated depending on the environmental conditions. Since the literature as well as the scientific knowledge on surface resistance is sparse, a simple model is introduced which describes the soil resistance r_{soil} in terms of path length and diffusivity:

$$r_{soil} = \frac{z}{D_{eff}} \quad (15)$$

where

$$\begin{aligned} D_{eff} &= \text{the effective diffusion coefficient in } m^2 s^{-1} \\ z &= \text{the dry soil layer in m} \end{aligned}$$

Several formalisms describing the dependence of D_{eff} on the free pore space in soil Φ_p are reviewed in /6/. Principally the relationship between the effective diffusivity D_{eff} , the diffusivity D_0 and the free pore volume Φ_p seems to be in the form of

$$D_{eff}/D_0 = a\Phi_p^b \quad \text{or} \quad D_{eff}/D_0 = a\Phi_p + c \quad (16)$$

where

a,b and c = constants for a specific type of material.

However, in our case an opposite behaviour of D_{eff} is recommended.

D_{eff} should decrease if Φ_p increases => high resistance

D_{eff} should increase if Φ_p decreases => low resistance

From that point of view the following relationship is introduced:

$$D_{eff} = D_0 \times \left(\frac{T_a}{273} \right)^{1.75} \times \frac{1}{\left(\frac{\Phi_m - \Phi_w}{\Phi_w} \right)} \times tort \quad (17)$$

where

$$\begin{aligned} D_0 &= \text{the diffusion coefficient of water vapour in air } (0.23 \times 10^{-4} m^2 s^{-1}) \\ T_a &= \text{the actual temperature in Kelvin} \\ \Phi_m &= \text{the maximum water content in the first cm in vol \%} \\ \Phi_w &= \text{the actual water content in the first cm in vol \%} \\ tort &= \text{the tortuosity factor } (tort = 1.5) \end{aligned}$$

The first part of this equation describes the dependency of the diffusion coefficient on the temperature whereas the second part controls diffusivity due to the water content in soil.

Theoretical considerations and some practical analysis /32/ show that for calculating the soil resistance, the water content in a soil layer of 0.5 to 1 cm depth is decisive. UFOTRI considers only a first soil layer of 5 cm depth. Therefore a so-called 'help layer' with the recommended depth of 1 cm is introduced into the code. The water content of this upper layer is calculated in a simple manner; it increases in case of rainfall and decreases by evaporation. Water transport due to matric forces is neglected. To consider the varying depth of the 'dry' soil layer z , the following approach is used:

$$z = z_0 / \Phi_h \quad (18)$$

where

- z_0 = the initial depth of the dry soil layer in m (0.004)
 Φ_h = the actual water content in the top first cm in mm water
 (limited in the program to values between 0.5 and 5)

In addition, a minimum resistance r_{sm} (which may be changed by the user) is introduced because a zero resistance seems to be unreasonable, also if the soil is saturated with water. Thus the actual resistance formula is:

$$r_{soil} = \frac{z}{D_{eff}} + r_{sm} \quad (19)$$

where

- r_{sm} = the minimum resistance of a wet soil surface

A comparison of the resistance model implemented in UFOTRI with two others described in /32/ and /5/ is shown in Figure 3.

The models of /32/ and /5/ are based on experimental data (lysimeter measurements). The evapotranspiration rate is fitted against a bulk resistance to determine the unknown soil resistance. The atmospheric resistance was calculated previously. The model according to Camillo et al. /5/ uses a linear dependence of the resistance on the soil moisture content whereas the model of Shu Fen Sun /32/ shows a highly nonlinear behaviour. Coming from a more simple approach one may define first the basic conditions for a resistance model which have to be fulfilled anyway: for a high water content in the first cm of the soil the resistance seems to be very low or nearly zero, and if the soil water content in the first cm is low, the resistance tends to increase to very high values. The shape of the resistance curve in between seems not to be well defined. The curve of the UFOTRI submodel looks more like the results of the model from Shu Fen Sun and meets the basic dependencies. However, because of the lack of knowledge about exact parametrization of soil resistances, further investigations are required, to decide whether a linear or a non-linear relationship of the soil resistance in dependence of the volumetric soil moisture content is adequate.

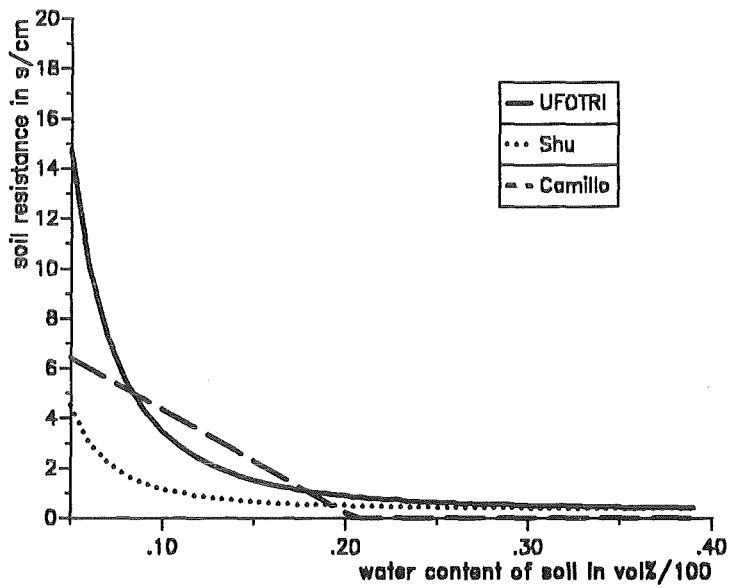


Figure 3. Comparison of 3 different soil resistance models

As a first test of the soil-water model including the new resistance approach, a model comparison with experimental data, measured at a site near Karlsruhe has been performed (Fig. 4 to Fig. 7).

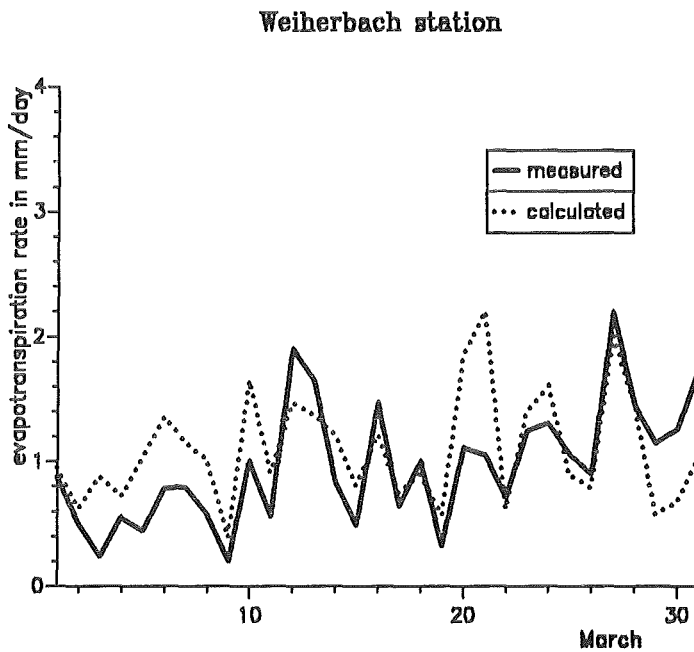
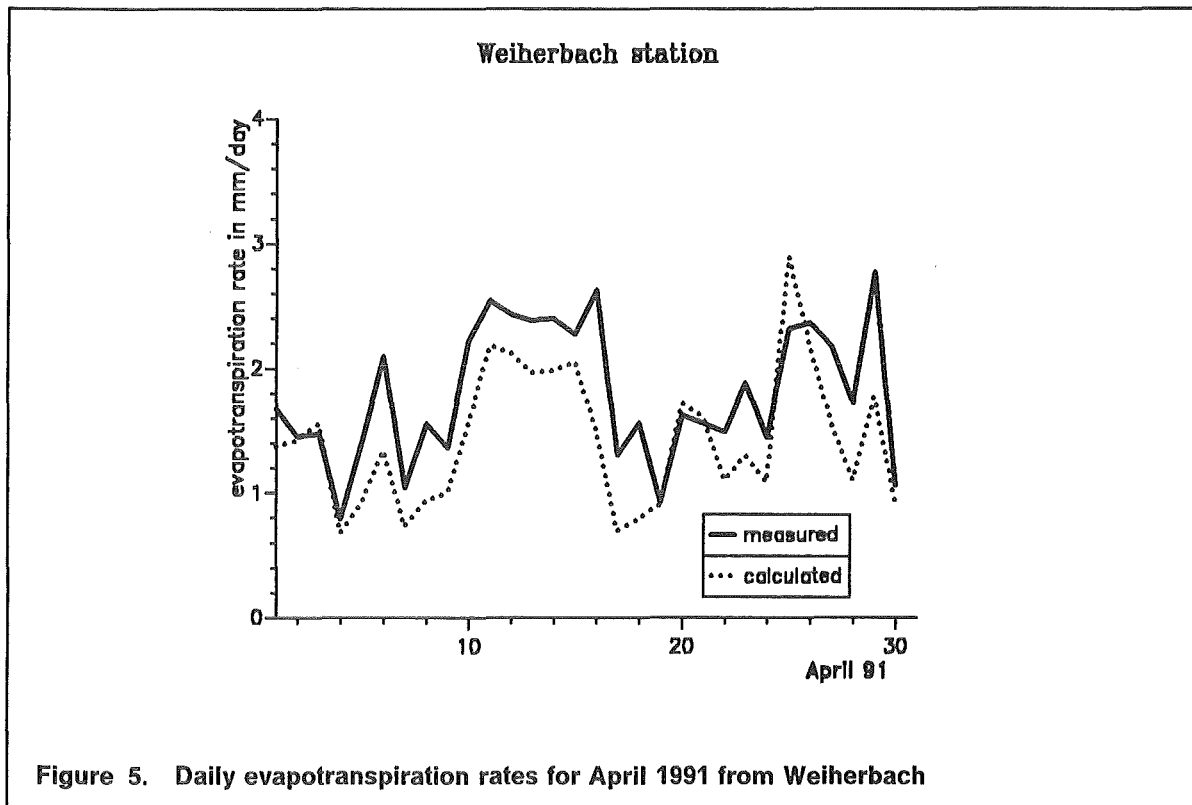
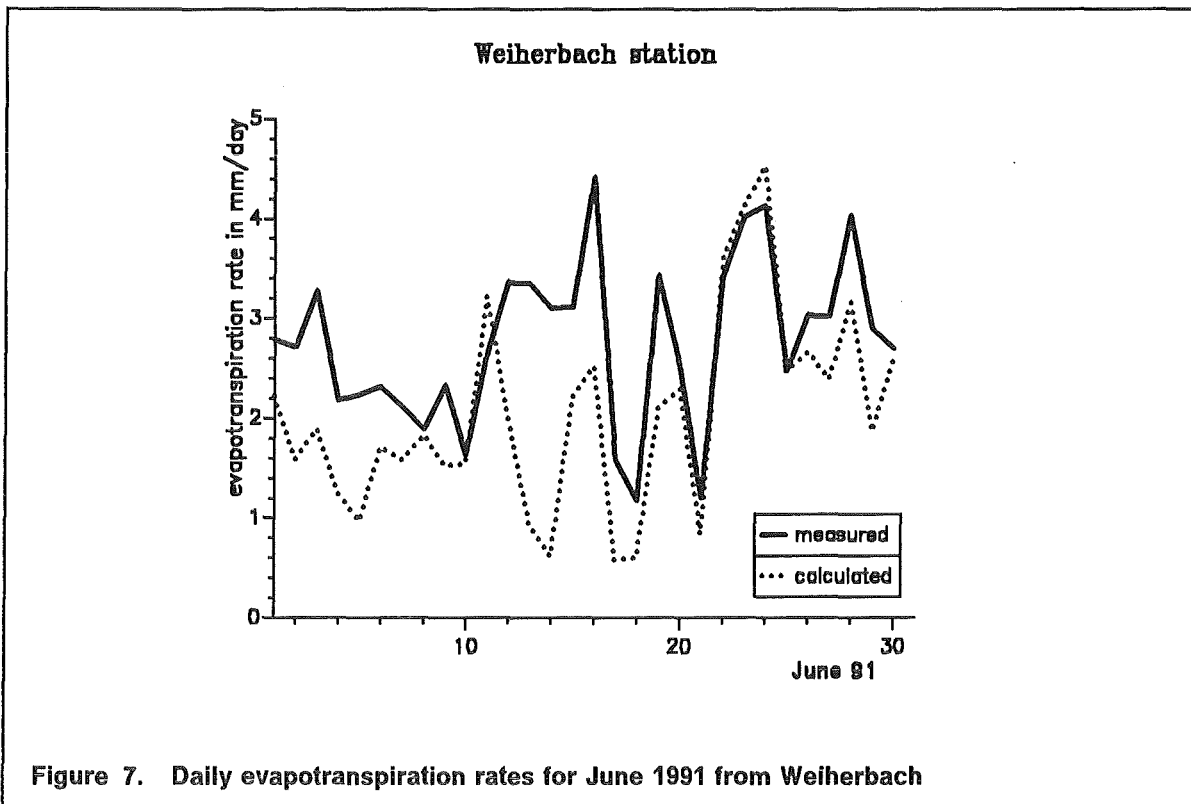
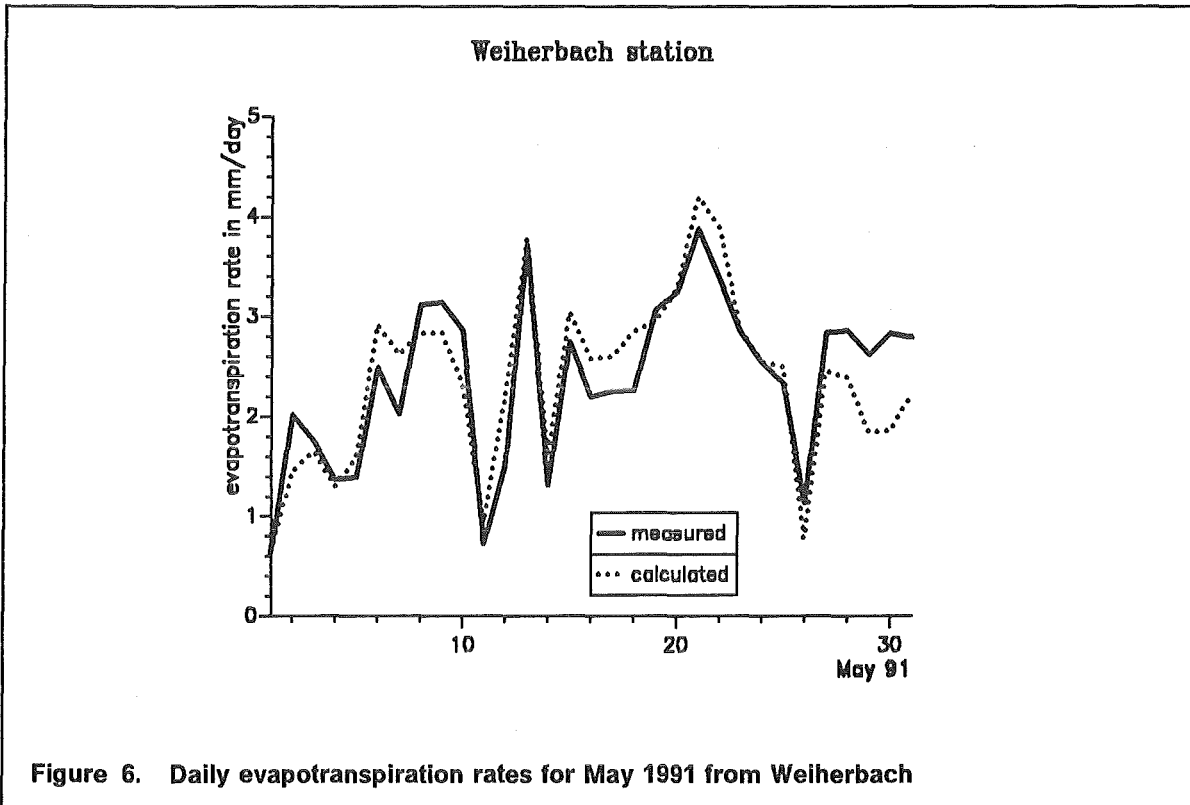


Figure 4. Daily evapotranspiration rates for March 1991 from Weiherbach

In general, the accordance of measured and calculated evapotranspiration rates are rather good. But in case of rain events (for example March 10, and April 25) the model overpredicts the measurements up to a factor of two. For these events, the evaporation from the soil is the dominating factor.





5.3.3 Wet deposition of tritium to soil (including derivation of soil resistance)

The process of wet deposition of HTO to soil is considered in the model as washout from the whole plume. The washout coefficients depend on the intensity of precipitation. They are very small for HT, i.e. wet deposition is neglected. UFOTRI offers two possibilities to calculate the wet deposition rate of HTO. In the first and recommended one, the washout coefficient is dependent on the precipitation intensity according to the following power law:

$$lam_{HTO} = AW \times I^{BW} \quad (20)$$

where

- lam_{HTO} = washout coefficient
- AW, BW = constants (9.0 10⁻⁵, 0.6)
- I = precipitation intensity in mm/h

The second possibility is to use precalculated whashout coefficients each representing one of 3 precipitation intensity classes (< 1 mm/h; 1 to 3 mm/h; > 3 mm/h).

5.3.4 Tranport of water and tritium in soil

The water content in the soil will increase in case of rain and will decrease as a result of evapotranspiration of plants and soil. Two different soil-water transfer models are available. In the simple version, water transport will occur only if the influx from precipitation exceeds the maximum water uptake capacity. In the more complex version, transport of water between each layer due to matric forces is considered. Therefore the hydraulic conductivity and the suction tension of the soil (the soil parameters should be representative of the whole area, if possible) are calculated according to the formulas proposed in /38/. The suction tension S in mm of water is given by:

$$S = 1.5 \times 10^5 \Psi^a + b\Psi + c\Psi^n \quad (21)$$

with

$$\Psi = \frac{(\Theta_s - \Theta)}{(\Theta_s - \Theta_w)} \quad (22)$$

where

- Θ_s = maximum water content in each soil layer in vol %,
- Θ_w = water content in each soil layer if the wilting point is reached in vol %,
- Θ = actual water content in each soil layer in vol %
- a, b, c, n = constants for a given soil.

The suction-conductivity function K in mm/d is defined as:

$$K = \frac{\alpha_q}{S^m + \beta} \quad (23)$$

where

α_q, m, β = soil specific constants

Applying a simplified version of Darcy's law leads to an expression for the moisture transfer from layer a to layer b:

$$V_{ab} = K_{ab} \left[\frac{(S_a - S_b)}{(\Delta z_a + \Delta z_b) / 2} - 1 \right] \quad (24)$$

where

V_{ab} = moisture transfer from layer a to b in mm/h

$\Delta z_{a,b}$ = diameter of soil layer a, b in mm.

Coupled with the water movement, a certain amount of tritium with its specific activity is transported from one layer to the other.

After having obtained the actual transpiration rate and the specific concentration of tritium in soil the uptake of HTO by the plant root system is calculated. To compensate the loss of water due to evaporation in the atmosphere, the roots of agricultural plants take up water, and thus also HTO, from soil layers up to a depth of 30 cm. For the model, it is assumed that 20% (40%) of the water taken up by the plant (grass) contains HTO with the specific concentration of the top 5 cm of the soil. The remainder of the water taken up by the plant is assumed to have a specific HTO concentration of deeper soil layers. In case of grass, 60% are taken from the second soil layer (5-15 cm). In case of the agricultural plants, the remaining 80% of water uptake comes equally from layer 2 (5-15 cm) and layer 3 (15-30 cm).

As mentioned above, the reemission rate of HTO from the plants is described by the model of Belot. The reemission rate of HTO from the soil during the daytime is coupled to the soil evaporation rate by an additional conversion factor which describes the differences of tritium and water behaviour. Additionally a basic reemission rate is introduced due to diffusion processes. The sum of both gives the effective reemission rate during the daytime. The reemission rate for conditions without insolation (night-time) is set to the basic reemission rate, which was derived from the Canadian field experiment /3/. The resulting reemission rate (basic value without insolation plus the daytime value) decreases with time after release (this is to account for the variation in the concentration difference between atmosphere and soil).

$$REEM = \frac{E_{as}}{BODWA} \times C_1 \times C_2 \times ZT + REB \times ZT \quad (25)$$

where

REEM	= reemission rate in % per hour
REB	= basic reemission rate in % per hour
E_{as}	= actual evaporation in $kg\ m^{-2}\ h^{-1}$
BODWA	= actual water content in the top soil layer in $kg\ m^{-2}$
C_1, C_2	= constants
ZT	= reduction of the initial reemission rate in dependence of the time after the release (exponential decrease)

During night-time the reemission rate is set to the constant value REB.

5.4 Modelling of the plant growth

In the present version of UFOTRI a model is introduced which simulates the time dependence of the leaf area index (LAI), the dry matter content of plants (potatoes and wheat), the water content of plants (potatoes and wheat) and the translocation of OB into the seed of winter wheat and the tubers of potatoes.

The developing stage of a nutriment plant is divided into three parts. After sowing, the plant will start growing and the content of organic material will reach a nearly constant value after several weeks. The full grown stage will held on for about several weeks. In this time the seedlings (wheat) and tubers (potato) will be mainly developed. Thereafter the senescent period starts and the plant is going to dry up. The leaf area index will go towards zero and the transfer rate into the organic matter especially in the edible parts decreases.

The growing period - time to reach the maximum water content, maximum organic matter content and maximum LAI of the plant - depends on the plant species. For winter wheat, the growing period starts in the early springtime (in the model at day 110) and ends at the beginning of summer (in the model at day 165). The development of potatoes is assumed to start in the middle of spring, (in the model at day 140) and ends in the early summer (in the model at day 170). The duration of the maximum developed stage of the plant will be 5 weeks and 8 weeks for winter wheat and for potatoes, respectively. Thereafter the plant will dry up until the day of harvest which is defined in the model as day 225 and day 258 for winter wheat and for potatoes, respectively. The overall time of biological activity is assumed to be about 120 days for both plant species. The growing period of the edible parts are 90 days for potatoes and 60 days for winter wheat.

All the times concerning the development stage of the plant, and the plant weights (see Table 1) are mean values valid for Germany. The weight values for the full grown plant stage have been derived from German literature. These values together with the harvesting time (but not the duration of the growing period) may be changed as model input. After having gained more experience with the new model version and when it will be

applied to different climatic regions, also the values for the growing period will be coded dynamically. This has some implications for the photosynthesis model (for example maximum photosynthesis rate per hour) described in the following. If all the dependencies are better understood a new release of UFOTRI may contain an extended plant model.

	leafy veget- ables	grass	potatoes	winter wheat
total plant matter	1600g /8/	850g /35/	3000g /30/	2500g /35/
dry matter plant	160g /34/	170g /8/	600g /7/	500g /7/
water content plant	1440g /34/	680g /8/	2400g /34/	2000g /7/
total matter fruits			3000g /35/	600g /35/
dry matter fruits			660g /34/	519g /34/
water content fruits			2340g /34/	81g /34/

Table 1. Key values for the developing stage of the plants considered in UFOTRI

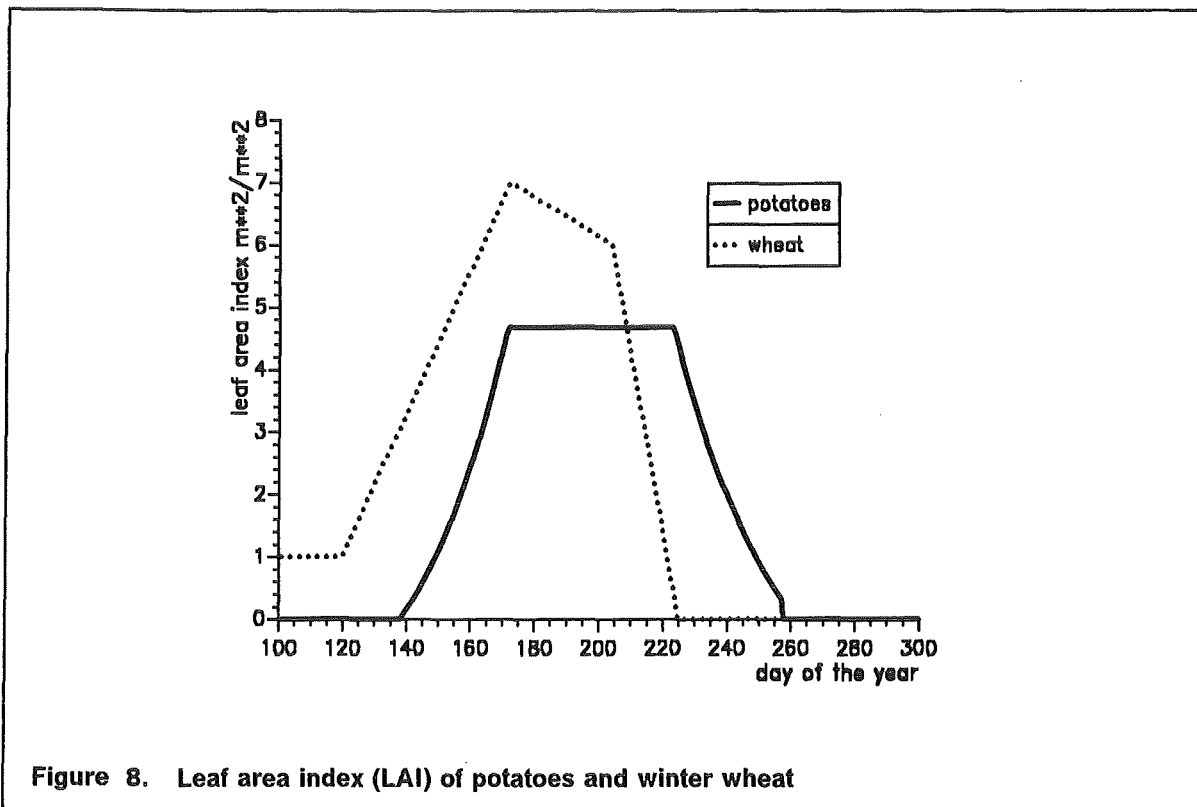


Figure 8. Leaf area index (LAI) of potatoes and winter wheat

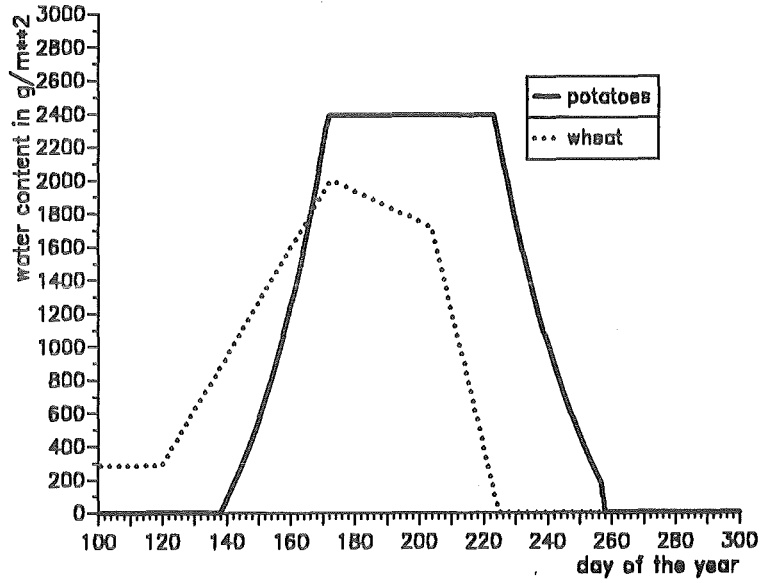


Figure 9. Water content of potatoes and winter wheat (in g)

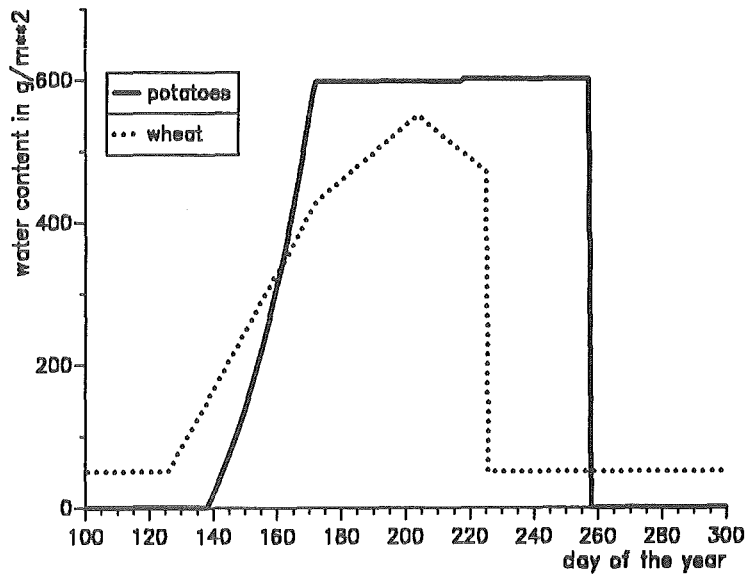


Figure 10. Content of organic matter for potatoes and winter wheat (in g)

5.5 Non-exchangeable tritium (including photosynthesis model)

5.5.1 Photosynthesis model

Since the edible parts of the plant will be harvested (thereafter consumed) - in general - many days after the release, the nonexchangeable bound tritium (OBT) is of importance for the dose assessment. OBT is the tritium form which is permanently bound within a carbon complex (organic matter). The dominating way to build up organic material is the photosynthesis process. In the 'old' model, the OBT uptake rate is only divided into an increased daytime (photosynthesis) and a reduced night-time value /15/. In the present UFOTRI version the translocation of OBT is based on a simple photosynthesis model. For leafy vegetables and grass the whole plant is considered, for winter wheat only the transfer into the seedlings and for potatoes only into the tubers is modelled by the photosynthesis model. To subdivide the daily values into hourly rates the incoming photosynthetic active radiation (PAR) and the status of the plant stomata have to be taken into account.

The photosynthesis rate is based on the amount of CO_2 assimilation under consideration of a conversion factor of 1.5 for the build up of organic matter /39/. The commonly used basic equation for net CO_2 assimilation, including respiration, without limiting factors in the hyperbolic form (/13/ and /31/) is:

$$P_{pot} = \frac{P_m \varepsilon I_{abs}}{P_m + \varepsilon I_{abs}} - Rd \quad (26)$$

where

- P_{pot} = potential CO_2 assimilation rate in $g CO_2 m^{-2} h^{-1}$
- P_m = the maximum CO_2 assimilation rate in $g CO_2 m^{-2} h^{-1}$
- I_{abs} = the absorbed photosynthetically active radiation in $W m^{-2}$
- ε = the initial light use efficiency in $g CO_2 W^{-1} h^{-1}$
- Rd = respiration rate in $g CO_2 m^{-2} h^{-1}$

To integrate this formula over the total depth of the crop canopy, it is assumed, that the PAR absorbed per leaf area decreases exponentially with leaf area depth L. Thus the PAR absorbed by the leaves in a certain depth is:

$$I_{abs} = I_{n0} \times k e^{-kL} \quad (27)$$

where

- I_{n0} = the incoming PAR in $W m^{-2}$
- L = the leaf area in m^2/m^2 , ranging from zero to LAI
- k = the extinction coefficient (0.6)

The analytical solution of equation 26 by using equation 27 results in a total canopy assimilation P_c of:

$$P_c = \frac{P_m}{k} \times \ln\left(\frac{P_m + \varepsilon k I_{n0}}{P_m + \varepsilon k I_{abs}}\right) - R_d \quad (28)$$

To take into account the dependence on the temperature, the maximum assimilation rate P_m has to be corrected. The original equation from /39/ has been slightly modified to adapt the calculated maximum value with recorded data from the literature (e.g. /20/).

$$P_m = \frac{0.158 \times C_0 \times 10^9 T \exp\left(-\frac{\Delta H_1}{RT}\right)}{1 + \exp\left(-\frac{\Delta H_2}{RT}\right) \exp\left(-\frac{\Delta S}{R}\right)} \quad (29)$$

where

- $\Delta H_1, \Delta H_2$ = the activation and denaturation energies for the electron transport in cal per mol
- C_0 = value for the build up of organic matter in $mg CO_2 m^{-2} h^{-1}$, plant species dependent
- R = the gas constant in cal/K per mol
- ΔS = the entropy change on denaturation of the electron transport system in cal/K per mol
- T = the air (leaf) temperature in Kelvin

The total respiration rate R_d of the plant species is defined by /21/:

$$R_d = C_{1_{Rd}} P_c + C_{2_{Rd}} W \quad (30)$$

where

- P_c = the CO_2 assimilation rate in $g CO_2 m^{-2} h^{-1}$
- W = dry matter of plant in the CO_2 equivalents / m^2
- $C_{1_{rd}}, C_{2_{rd}}$ = constants

The dependences of $C_{2_{Rd}}$ on the air temperature and the amount of accumulated biomass have been neglected. Values of the constants $C_{1_{Rd}}$ and $C_{2_{Rd}}$ used in UFOTRI are adopted from /21/.

- $C_{1_{Rd}} = 0.36$
- $C_{2_{Rd}} = 1.67 \cdot 10^{-4} g/h$ per $g CO_2$ equivalent

P_c and W' are expressed in CO_2 equivalents.

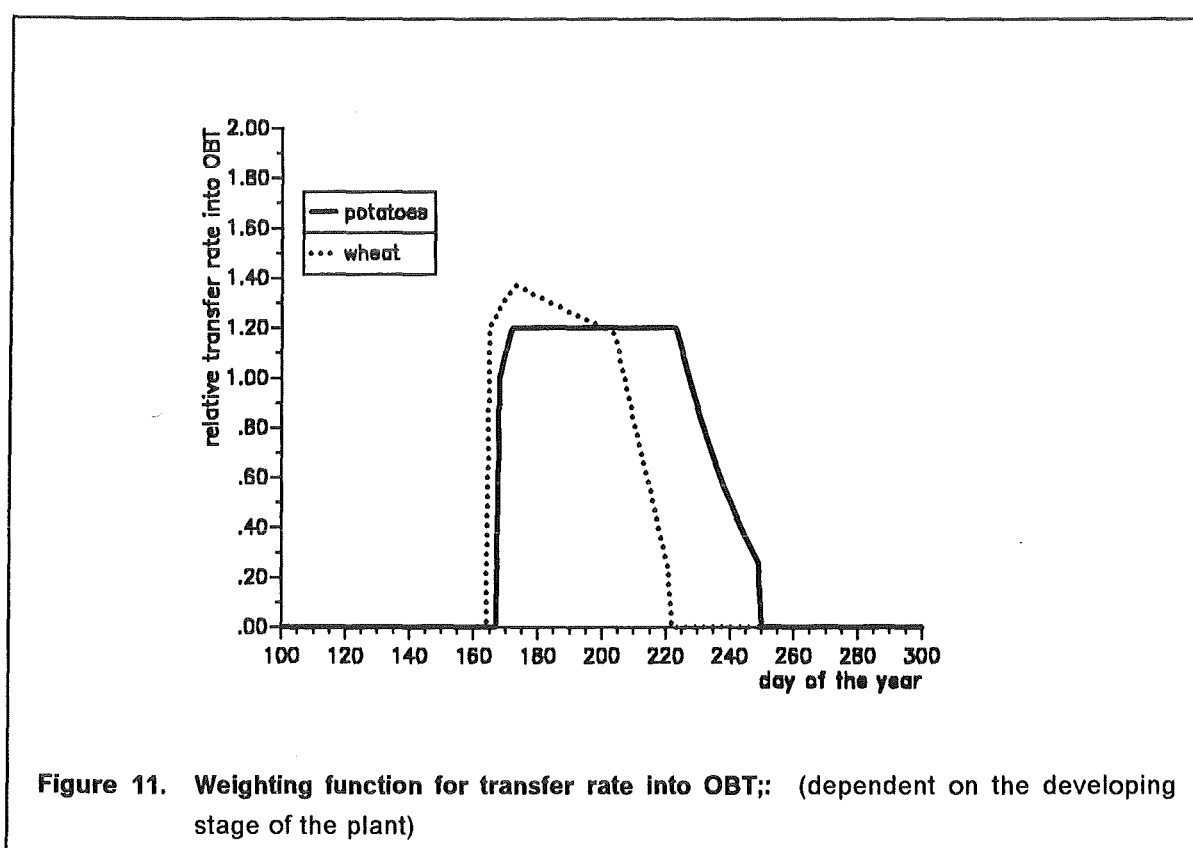
The reported formulae are valid for a plant without any stress factors growing under optimal conditions /39/ and /20/. To account for the stomata responses due to changing environmental conditions, the weighing factors for the stomatal resistance (derivation see chapter 2.2) have been applied. Thus the actual photosynthesis rate is expressed as:

$$P_{act} = P_c \times COA \times f(r) \quad (31)$$

where

- COA = conversion factor CO_2 to dry matter (1.5)
 f(r) = the weighting function due to solar insolation, air humidity,
 air temperature and water content in the soil

Applying equation 31 to winter wheat, using the meteorology of one year, representative for Karlsruhe, and assuming that irrigation occurs if the soil water content drops below a certain threshold, a build up of about $1800g$ dry matter m^{-2} will be reached at harvesting time; assuming no irrigation, the dry matter content is about $900g$. This corresponds relatively well to the mean total dry matter of about $1000g$ listed in table 1.



5.5.2 Transfer HTO into OBT

UFOTRI offers two possibilities to calculate the transfer of tissue free water tritium into organically bound tritium. The first and recommended one is the use of the photosynthesis model which allows for the calculation of an hourly photosynthesis rate, dependent on the environmental conditions. The second one is to use a mean uniform photosynthesis rate. The calculation procedure itself passes through several steps. The first step is identical for both calculation methods. The second step is the endpoint of the 'simple' model whereas the third step is the endpoint of the recommended model.

1. Determination of a uniform transfer rate into OBT.

- Calculation of a uniform transfer rate T_m (1/d) dependent on equilibrium conditions (see chapter 3 for further details about the derivation of transfer rates; for grass: $T_m = T_{5,8}$, for leafy vegetables: $T_m = T_{14,15}$, for potatoes: $T_m = T_{p5,p8}$, for wheat: $T_m = T_{w5,w6}$)

2. Simple model: Modification of the uniform photosynthesis rate dependent on the developing stage of the plant and the daylight / night period.

- The modification factor is presented in Figure 11. The integral over the uniform (fact1 = 1) and the modified factor is equal.
- The modification factor fact2 depends on daylight or night periods (explanation see later on)

$$T_{act} = T_m \times fact1 \times fact2 \quad (32)$$

where

T_{act} = the actual transfer rate of HTO into OBT in 1/h

T_m = mean hourly transfer rate into OBT in 1/h
(derived from the daily value)

fact1 = weighting factor from Figure 11

fact2 = weighting factor day / night (1.75 / 0.25)

3. Advanced model:

- Calculation of a mean uniform photosynthesis rate for grass, vegetables, the tubers of potatoes and seedlings of winter wheat.

With a growing time of 30 and 45 days for grass and vegetables, respectively, and the dry weight from Table 1, a mean uniform dry matter build up rate can be derived.

The dry matter content of tubers and seedlings taken from Table 1, together with the developing times of 90 and 60 days, respectively, give the mean uniform dry matter build up rate for potatoes and wheat.

- Calculation of an hourly photosynthesis rate which is directly coupled to an hourly transfer rate into OBT. The actual hourly (calculated with equation 31) photosynthesis rate P_{act} will be divided by the uniform photosynthesis rate $P_{m,f}$, thereafter multiplied with the mean uniform transfer rate T_m and a distribution factor, describing the nonuniform tritium distribution in the plant. This leads to the following equation:

$$T_{act} = \frac{P_{act}}{P_m} \times T_m \times fact2 \times dis \quad (33)$$

where

- P_{act} = actual hourly dry matter production rate in g/h
 P_m = mean hourly dry matter production rate in g/h
 (12 hours per day growing period)
 dis = factor describing the nonuniform distribution of HTO in plant
 (default = 0.5)

The distribution factor is introduced in the model, because the tritium distribution in the plant (in the nature) is nonuniform, but is assumed to be uniform in the model. Since some parts of the plants are more important for the OBT production than others (first leaf for example) the introduction of a distribution factor makes the model more flexible. After the evaluation of the plant experiments which are under way at KfK /7/, 'realistic' values for the distribution may be found. The present default value is the result of first evaluations of some experiments. The specific tritium concentration (Bq/g) of the organic matter of the edible parts of wheat or potatoes contains about 0.1 to 0.5 percent of the specific HTO concentration (Bq/g) taken up by the plant after the exposure has been stopped /7/.

Until now the OBT transfer model is only physically founded for the hours with solar insolation. During the night it is assumed, that the transfer rate is a quarter of the daily mean. Thus the 'light' transfer rate has to be multiplied with 1.75 to meet the daily integral value of 1 (values can be found in fact2). A detailed modelling of the night-time period is not realized due to the lack of knowledge and data. Thus the 'one fourth' assumption was adopted - but slightly modified - from the literature /22/. Ongoing experimental work may help to close this gap of knowledge.

A loss out of the organic tritium compartment is observed as well. Assuming an exponential concentration decrease in the OBT compartment, a mean loss rate of some tenths of a percent per hour is assumed in the model. A loss of OBT from the edible parts of the wheat plant (seedlings) and the potato plant (tubers) is not allowed.

5.6 Cow compartment

In the atmospheric part of UFOTRI, all exchange processes cow/atmosphere, cow/plant and cow/soil, which are important for the ingestion pathways via milk, beef and dairy products, are also considered. The transfer rates are in general the same as for the ingestion module of UFOTRI, which were derived on the basis of a constant daily rate, but now converted to an hourly value. This shortening of the time step allows to model

some processes more accurately. So the cows ingest their pasture grass only during the daytime. Furthermore the cows do not produce milk continuously but they are usually milked two times a day, once in the morning and once in the evening.

5.7 Dose calculations

The incorporation of HTO by inhalation is calculated with an average breathing rate, averaged over the daily normal activities of an average individual of the corresponding population group and assuming that all tritium is resorbed in the body. The divergent behaviour of HT is described by a reduced dose conversion factor of about four orders of magnitude. Skin absorption is taken into account by an additional absorption rate of HTO from the air.

$$D_{IH} = (BR + SKR) \times DCF \times C_{a,t} \quad (34)$$

where

- D_{IH} = dose from inhalation and skin absorption in Sv
- BR = breathing rate in $m^3 s^{-1}$
- SKR = skin absorption rate in $m^3 s^{-1}$
- DCF = dose-conversion factor in Sv/Bq
- $C_{a,t}$ = time-integrated air concentration in $Bq sm^{-3}$

For estimating the individual intake from the ingestion pathways, the conservative assumption is made that all food consumed is produced locally. From the intake the dose can be obtained with dose factors to convert the ingested activity into dose.

The food products which have to be considered in the foodchain model are chosen according to their significance for the consumption habits of the population. Most of the foodstuffs can be assigned to the three classes:

- vegetable products
- meat and meat products
- milk and milk products

From the first class, leafy vegetables, potatoes and winter wheat are taken as representative foodstuffs and are considered in the program. Beef from a cattle and milk from a dairy cow are chosen as representative for the other two classes. In the program, both chemical forms of the ingested tritium, OBT and HTO, are calculated separately for the plant-, cow- and milk-compartments. Thus individual dose-conversion factors for HTO and OBT are considered separately in the model. The dose results by summing up the incorporated activity of the relevant foodstuffs.

$$D_{IN} = \sum_{f=1}^2 DCF_F \times \sum_{N=1}^5 IG_N \times C_{N,F} \quad (35)$$

where

- D_{IN} = dose from ingestion
- N = foodstuff: milk, meat, vegetables, potatoes, grain products
- F = chemical form of tritium (HTO or OBT)
- DCF_F = dose-conversion factor (HTO, OBT) in SV/Bq
- IG_N = consumption rate of foodstuff N in $kg\ d^{-1}$
- $C_{N,F}$ = time-integrated specific concentration in the foodstuff N in $Bq\ dkg^{-1}$

The present version contains a submodel which allows for the consideration of food restriction when calculating the ingestion dose. Restrictions are based on the tritium level in food on a fresh weight basis. The user can input a value for each foodstuff (default = 1250 Bq/kg) separately.

The collective dose may be calculated by multiplying the individual dose value with the population living in the area represented by a single grid point.

6. Extensions and changes in the long term ingestion module of UFOTRI

6.1 Overview

In this part of the model, the long term behaviour of tritium in the environment and the assessment of the long term doses of the population from the consumption of tritium contaminated foodstuffs are described. To that purpose, the model calculates the actual concentration at the time of harvest in potatoes and grain and the time integrated tritium concentrations in vegetables, meat and milk products. The dose resulting from the uptake of drinking water is in general negligibly small because of the dilution processes of tritium in rivers, lakes and ground water, before it may be used for consumption.

To consider all relevant components of the foodchains and their link to the dispersion module (Fig. 1 and Fig. 2), it was again necessary to subdivide the whole complex into two parts, corresponding to the production of nutriment plants only (leafy vegetables, potatoes and wheat) and for production of milk products and meat. The nutriment plants are subdivided - if necessary - into three parts, one for the bulb below the surface, one for the body of the plant and one for the fruits. The complicated exchange processes between plant soil and atmosphere and the great variability of plant species do not allow to consider them all in detail, in particular with regard to the unacceptable computer time required by such a model.

To describe the transport processes mathematically, the areas in the environment where tritium may appear are divided into different compartments as shown in Fig. 2. A compartment is an idealized range of the environment in which specific material can be enriched or diluted by exchange processes. The transfer rates which quantify the transfer processes are averaged values valid for longer periods and calculated assuming equilibrium conditions. The exchange processes between the individual compartments are treated by first order differential equations which describe linear dependences of tritium concentrations or concentration differences. The system of differential equations resulting from many compartments of the foodchain models cannot be solved analytically. Accordingly, the computer model COMA (Compartment Model Analysis) developed at NRPB (National Radiological Protection Board, UK), was chosen to solve the problem numerically /29/ .

The basic reference /24/ contains detailed information about the long term ingestion module. The procedure how to calculate the individual transfer rates have not been changed since the report from 1991. However, most of the values of the transfer rates have been changed due to their dependence on the mass content of the compartment. The revised inventory (water content and content of organic matter) of the plants under consideration are listed in Table 1. It does not seem to be useful to present here the derivations of all the transfer rates considered now in the model, because the principles

of the exchanges remain the same as in /24/, only the values have been up-dated. Two new nutriment plants have been identified to be important for the dose calculations from the ingestion pathways. The consideration of new plant species such as potatoes and winter wheat necessitates new transfer pathways, to meet better the physical reality. Therefore it was necessary to subdivide the plant into an edible part (tuber for potato and seedling for wheat) and a nonedible part. The derivation of these new transfer paths and rates will be presented briefly in the following. A table with all transfer rates together with their default values (dependent on a standard input) is attached at the end of this report (Tab. 9 to Tab. 12). However, these values are not fixed since they will be reevaluated in every model run dependent on the choice of the input parameters.

6.2 Determination of the transfer rates

6.2.1 Introduction

To calculate the transfer rates the knowledge of different states of the compartment system must be available. If the equilibrium between two compartments is known, one can choose the transfer rates in a way, that under constant external conditions equilibrium is reached. In general, equilibrium conditions mean, that a compartment should not loose or take up any mass during the considered time period. The transfer rates are calculated on the basis of hydrogen inventory in and hydrogen exchange between the compartments. The following assumptions are made:

- Hydrogen content in water $\approx 11\%$
- Hydrogen content in the organic parts of the plant $\approx 8\%$
- Hydrogen content in the organic parts of the cow $\approx 8\%$
- Hydrogen content in the organic parts of the milk $\approx 8\%$

Furtheron it is necessary to define a mean mass content for each compartment. The transfer rates have the dimension d^{-1} ; they are all derived for one square km, but this normalization does not appear explicitly in the formulas.

6.2.2 Grass

The half time of loss from the organic compartment has been changed from 10 days to 15 days. This fits more the assumption, that the growing period of grass (for feeding) is about 30 days /12/. Thus the exchange rates from the organic compartment to the water compartment ($t_{6,5}$) and back ($t_{5,6}$) have been assigned new values (see Tab. 10).

6.2.3 Leafy vegetables

The half time of loss from the organic compartment of leafy vegetables has been changed from 10 to 22 days. The reason is that now a growing period of about 45 days is assumed for leafy vegetables, especially for salad /12/. This new value halves both transfer rates, namely $t_{15,14}$ from the organic to the water compartments, and $t_{14,15}$ from the water compartment to the organic compartment (see Tab. 9).

6.2.4 Potatoes

Potatoes are the first new plant introduced in UFOTRI. The transfer rates and pathways are shown in Table 11 and Fig. 12, respectively. The basis for the calculation of the transfers soil atmosphere ($t_{p1,p2}$ $t_{p2,p1}$), the transfers from one soil layer to the other ($t_{p2,p3}$; $t_{p3,p2}$; $t_{p3,p4}$; $t_{p4,p3}$ and $t_{p4,p4}$), and the transfers plant atmosphere ($t_{p1,p5}$ and $t_{p5,p1}$) remains the same as for leafy vegetables described in /25/. Modifications have become necessary because of the subdivision of the potato plant in an edible part (tuber) and a nonedible part (plant body). For the dose calculations only the tritium content in the tubers are of importance.

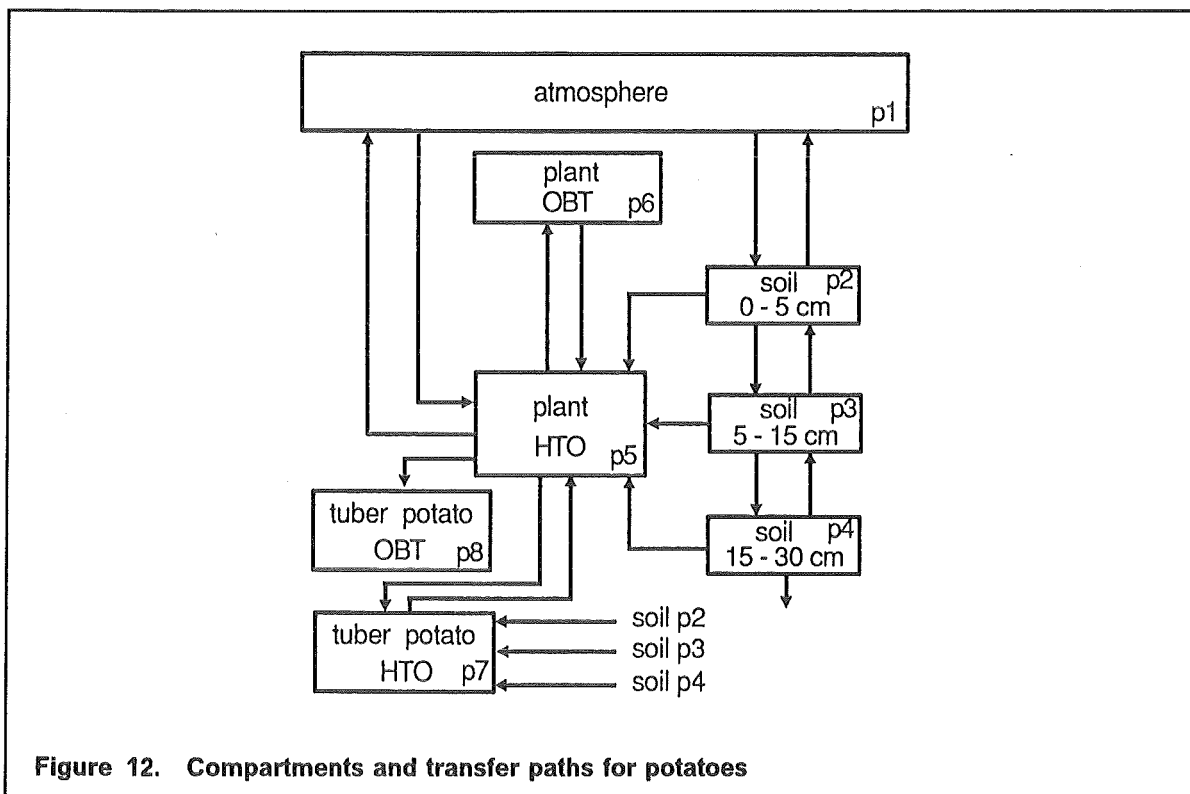


Figure 12. Compartments and transfer paths for potatoes

The basis for the determination of the root uptake of the potatoes is the assumption that the specific tritium concentration in potato plants at the state of equilibrium is half that of the atmosphere, if the tritium source is located therein. The other half enters the plant

from the soil (3 layers) via the root system. In the new model version the transfer from the three soil compartments to the plant is subdivided into two paths. One part of the water will reach the plant body directly whereas the other one goes into the tubers. Following the root uptake distribution as mentioned in /25/, the following contribution of the water from a soil layer to the plant is used:

- from soil-1 (0 - 5 cm) uptake of 20 %
- from soil-2 (5 - 15 cm) uptake of 40 %
- from soil-3 (15 - 30 cm) uptake of 40 %

The overall transfer rate will be calculated in the following manner.

$$t_{tot} = \frac{\text{uptake of plant (incl. tubers)}}{\text{hydrogen content of soil compartment}} \times \frac{\text{contribution factor in \%}}{100} \quad (36)$$

The overall transfer rate will be subdivided into:

- 5/6 reaches the plant body
- 1/6 reaches the tubers

This division has to be discussed in the future and is the result of a first understanding of the process.

Transfer rate $t_{p2,p5}$ soil p2⇒plant

$$\begin{aligned} t_{p2,p5} &= \frac{t_{p5,p1} \times M_{pot,w} \times 0.5 \times 5/6}{12.5} \times 0.2 \\ &= 4.4 \cdot 10^{-2} d^{-1} \end{aligned} \quad (37)$$

in which

$$M_{pot,w} = \text{Water content of the potato plant}$$

Transfer rate $t_{p3,p5}$ soil p3⇒plant

$$\begin{aligned} t_{p3,p5} &= \frac{t_{p5,p1} \times M_{pot,w} \times 0.5 \times 5/6}{25.0} \times 0.4 \\ &= 4.4 \cdot 10^{-2} d^{-1} \end{aligned} \quad (38)$$

Transfer rate $t_{p4,p5}$ soil p4⇒plant

$$\begin{aligned} t_{p4,p5} &= \frac{t_{p5,p1} \times M_{pot,w} \times 0.5 \times 5/6}{37.5} \times 0.4 \\ &= 2.9 \cdot 10^{-2} d^{-1} \end{aligned} \quad (39)$$

The remaining 1/6 of the total plant uptake via the root system will remain in the tubers which defines the following transfer rates:

Transfer rate $t_{p2,p7}$ soil p2⇒tuber

$$\begin{aligned}
 t_{p2,p7} &= \frac{t_{p5,p1} \times M_{pot,w} \times 0.5 \times 1/6}{12.5} \times 0.2 \\
 &= 8.8 \cdot 10^{-3} \text{ d}^{-1}
 \end{aligned} \tag{40}$$

Transfer rate $t_{p3,p7}$ soil p3⇒tuber

$$\begin{aligned}
 t_{p3,p7} &= \frac{t_{p5,p1} \times M_{pot,w} \times 0.5 \times 5/6}{25.0} \times 0.4 \\
 &= 8.8 \cdot 10^{-3} \text{ d}^{-1}
 \end{aligned} \tag{41}$$

Transfer rate $t_{p4,p7}$ soil p4⇒tuber

$$\begin{aligned}
 t_{p4,p7} &= \frac{t_{p5,p1} \times M_{pot,w} \times 0.5 \times 5/6}{37.5} \times 0.4 \\
 &= 5.8 \cdot 10^{-2} \text{ d}^{-1}
 \end{aligned} \tag{42}$$

The transfer rates plant body to tubers are set by analogy to the transfers plant-atmosphere-soil. At equilibrium it is assumed that half of the water (tritium) comes from the soil and half of the water (tritium) comes from the plant body. Having defined the input from the soil to the tubers as 1/6 of the loss to the atmosphere (see derivation above) the transfer plant-tuber is defined as:

Transfer rate $t_{p5,p7}$ HTO plant⇒HTO tuber

$$\begin{aligned}
 t_{p5,p7} &= \frac{t_{p5,p1} \times 0.5}{6} \\
 &= 2.0 \cdot 10^{-1} \text{ d}^{-1}
 \end{aligned} \tag{43}$$

This assumption is a first approach and needs further discussions. There exists also some indications that most of the water which reaches the tubers comes from the soil only /7/.

Starting with an equilibrium state tuber-plant, the transfer rate from the tuber to the plant is the sum of all uptakes (via the plant body and via the roots).

Transfer rate $t_{p7,p5}$ HTO tuber⇒HTO plant

$$\begin{aligned}
 t_{p7,p5} &= \frac{t_{p5,p1} \times M_{pot,w} \times 0.5 \times 2/6}{M_{tub,w}} \\
 &= 4.7 \cdot 10^{-1} \text{ d}^{-1}
 \end{aligned} \tag{44}$$

in which

$M_{tub,w}$ = water content of the potato tuber

It is assumed in the model that the organic compartment of the potato tuber is a sink for tritium. The physical meaning is that all the organically bound tritium is fixed there in an insoluble form, which remains there also after the time of harvesting. After harvesting the tritium content in the water compartment of the tubers will also remain constant (no transpiration). Adopting a growing period for the tubers of about 90 days the transfer rate is:

Transfer rate $t_{p5,p8}$ HTO plant \Rightarrow OBT tuber

$$\begin{aligned} t_{p5,p8} &= \ln \frac{2}{\text{HWZ}} \times \frac{M_{tub,o}}{M_{pot,hw}} \\ &= 2.0 \cdot 10^{-2} \text{ d}^{-1} \end{aligned} \quad (45)$$

in which

- $M_{pot,hw}$ = hydrogen content of the potato plant
- $M_{tub,o}$ = hydrogen content of the tubers
- HWZ = half time of developing period of the tubers (45 days)

6.2.5 Winter wheat

The second new plant in UFOTRI is winter wheat. The transfer pathways are shown in Table 12. As described for potato plants, the basis of the calculations of the transfer rates soil atmosphere ($t_{w1,w2}$ $t_{w2,w1}$), the transfers from one soil layer to the other ($t_{w2,w3}$; $t_{w3,w2}$; $t_{w3,w4}$; $t_{w4,w3}$ and $t_{w4,w4}$), the transfers plant atmosphere ($t_{w1,w5}$ and $t_{w5,w1}$), and the transfers from soil to the plant body ($t_{w2,w5}$; $t_{w3,w5}$ and $t_{w4,w5}$) remain comparable to the general derivation performed for the vegetable plant. The transfer rates are listed in Table 12. The values have been generated with the standard input file containing the mass of organic and inorganic matter in the plants shown in Table 1.

In accordance with the considerations for potatoes, the wheat plant is subdivided into an edible (seed) and a nonedible part (plant body). For the dose calculations only the tritium content in the seed (edible part) is of importance.

Two compartments representing the organic and inorganic part of the seed together with its transfer paths and rates will be presented in the following. It is assumed, that the exchange between the plant body water compartment and the water compartment of the seed is relatively fast. This approach is based on measurements performed at KfK which are still under evaluation /7/. The half time of the transfer is set to 2 hours.

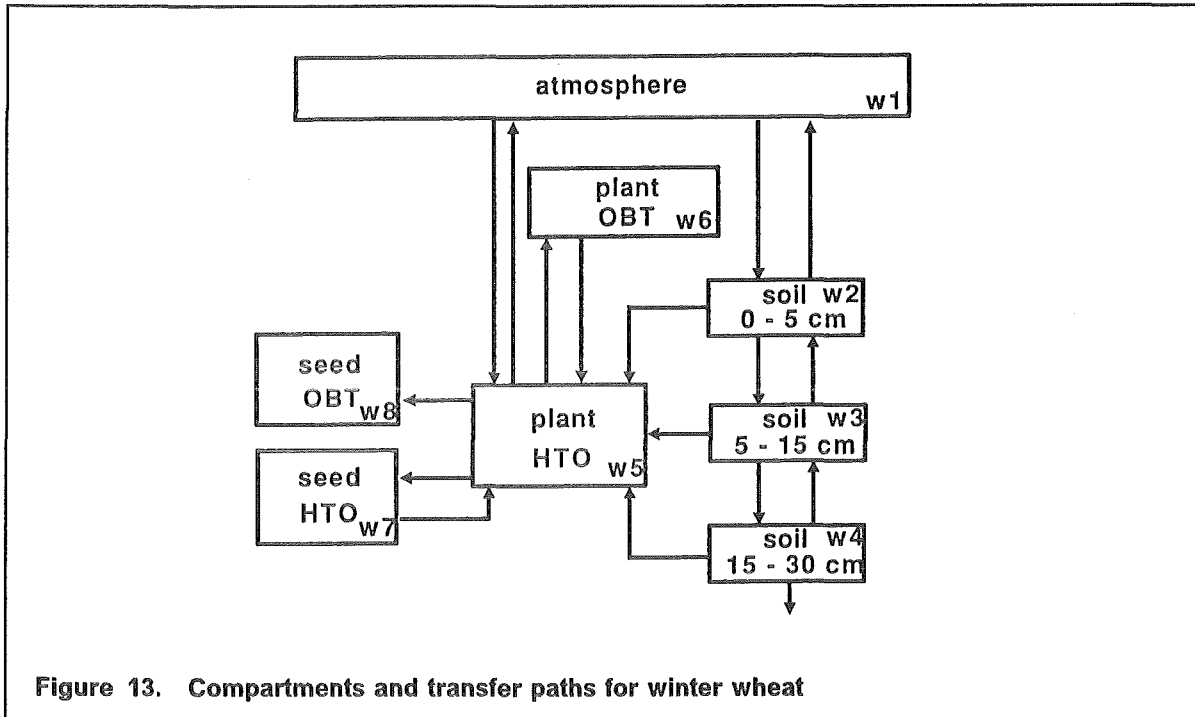


Figure 13. Compartments and transfer paths for winter wheat

Transfer rate $t_{w5,w7}$ HTO plant \Rightarrow HTO seed

$$t_{w5,w7} = 8.3 d^{-1} \quad (46)$$

This rate may be modified if the series of plant experiments performed at KfK have been analysed in total.

With the assumption of an equilibrium seed-plant the transfer rate from the water compartment of the seed to the water compartment of the plant body is:

Transfer rate $t_{w7,w5}$ HTO seed \Rightarrow HTO plant

$$\begin{aligned} t_{w7,w5} &= t_{w5,w7} \times \frac{M_{se,w}}{M_{whe,w}} \\ &= 3.2 \cdot 10^{-1} d^{-1} \end{aligned} \quad (47)$$

in which

$$\begin{aligned} M_{se,w} &= \text{water content of the seed} \\ M_{whe,w} &= \text{water content of wheat plant} \end{aligned}$$

As assumed for potatoes, the organic compartment of the seed is a sink for tritium. After harvesting, the tritium content in the water part of the seed remains constant (no transpiration). With a growing period of about 60 days the transfer rate is:

Transfer rate $t_{w5,w8}$ HTO plant \Rightarrow OBT seed

$$\begin{aligned} t_{w5,w6} &= \ln \frac{2}{HWZ} \times \frac{M_{tub,o}}{M_{pot,hw}} \\ &= 2.9 \cdot 10^{-2} d^{-1} \end{aligned} \quad (48)$$

in which

$M_{whe,hw}$ = hydrogen content of the wheat plant

$M_{sed,o}$ = hydrogen content of the seed

HWZ = half time of developing for the wheat seed (30 days)

7. Description of the input data defined by the user

7.1 General remarks

For most of the steering parameters defining the run and adapting the models to the user's needs, default values are given in UFOTRI. The input data are subdivided in several groups, identified by a title card. Only the input group TRIDAT has no title card. The group title cards have to be left justified. One part of the groups must always appears in the input data (obligatory input groups), the other part only if changes in the default values are wanted (optional input groups). The obligatory groups are entered in strict format, as described below. The optional groups are input using a FORTRAN NAMELIST. The ways in which NAMELISTs can be used are described in chapter 5.

The GROUP and NAMELIST names are:

GROUP	NAMELIST
Obligatory	
METEOZON	----
SOURCE	----
END	----
Optional	
PRINTOUT	OUTPAR
POLGRID	GRDPAR
ISOTOPE	ISOPAR
METEOROL	METPAR
----	TRIDAT

Obligatory input groups

- **METEOZON** data for the meteorological zone considered for the atmospheric dispersion calculation, the sampling of the weather sequences and the sites with their population data
- **SOURCE** data defining the release (thermal energy, release height, timing, etc.)
- **END** card at the end of the UFOTRI-specific input data

Optional input groups

- **PRINTOUT** options defining the paper output to be produced
- **POLGRID** definition of the polar grid
- **ISOTOPE** specifications of the nuclides considered, washout coefficient, deposition parameters
- **METEOROL** parameters for the atmospheric dispersion module (mixing layer height, wind profile, σ -parameters etc.) and the conditions for one single weather sequence chosen by the user (if METIN \neq 0)
- **TRIDAT** Tritium-specific input data for the atmospheric dispersion module and the longer term ingestion module

For the order of the input groups the following rules must be considered:

1. The group ISOTOPE must precede the group SOURCE.
2. The group POLGRID must precede the group METEOZON.
3. The group PRINTOUT must precede the group POLGRID.
4. The last group of the UFOTRI-specific input must be END.
5. If the NAMELIST TRIDAT is used, this card must appear after the group END.

The program unit INDAT gives a printout of the options and input data used for the run. In the following the input parameters of the NAMELIST groups are described. K means one or more input cards; S is a label for branching.

The type of the variables and arrays is given by the implicit FORTRAN type declaration; otherwise it is mentioned below.

Most of the arrays used have a dimension declarator defined by the PARAMETER statement. The maximum dimensions currently used in UFOTRI are shown in the table below. The statements are given in the member PARAM and are input to the code by the INCLUDE statement.

PARAMETER (NSITMX = 5, LWMAX = 144, NPHSMX = 17)

PARAMETER (NTYPMX = 2, NUCMAX = 2)

PARAMETER (NRMAX = 20, NPHIMX = 72)

```
*****
*
*   NSITMX   : MAX. NO. OF SITES           : = 5       *
*   LWMAX    : MAX. NO. OF WEATHER SEQUENCES : = 144      *
*   NPHSMX   : MAX. NO. OF RELEASE PHASES   : = 17       *
*   NRMAX    : MAX. NO. OF RADIAL DISTANCES : = 20       *
*   NPHIMX   : MAX. NO. OF ANGULAR SEGMENTS : = 72       *
*   NTYPMX   : MAX. NO. OF TYPE OF NUCLIDES : = 2       *
*           WITH DIFFERENT DEPOSITION      *
*           CHARACTERISTICS                 *
*   NUCMAX   : MAX. NO. OF NUCLIDES        : = 2       *
*
*****
```

7.2 Obligatory input groups

7.2.1 Input group METEOZON

The input group METEOZON specifies the selected meteorological zone and defines the data of the sites and of the weather sequences chosen for this zone.

The user can choose his own met-sampling program to generate site-specific weather sequences (read from NUNITS(13)) and similarly his own site-specific population grid (read from NUNITS(31)), or he can use the default options, for example cyclic sampling of weather sequences or a uniform population distribution.

- * If the grid differs from the default values the input
- * group POLGRID must precede the input of METEOZON

K1.1 title card METEOZON
(FORMAT A8)

METEOZON name of identification (left-justified)

K1.2 Card of the selected meteorological zone
(FORMAT 1X, A8, 1X, 2I10, 5I5)

ZONNAM name of the meteorological zone

LMAX number of weather sequences (max. LWMAX)

NSTMAX number of sites (max. NSITMX, not considered here)

LPOPT option for specifying the probabilities PWET of
the weather sequences
= 0 uniform distribution, i.e. $PWET = 1/LMAX$
≠ 0 PWET is defined by
= 1 the input list K1.4
= 2 the weather sequence data file (NUNITS(13))

LWOPT option for specifying the starting times LWET of
the weather sequences
= 0 cyclic sampling
≠ 0 LWET is defined by
= 1 the input list K1.3
= 2 the weather sequence data file (NUNITS(13))

IRAU index of surface roughness for the choice of the dispersion parameters
 = 2 mean roughnesslength (low plants, rural areas, length of roughness $Z < 10$ cm to 1 m)
 = 3 great roughnesslength (forests, urban areas, length of roughness $Z > 1$ m)

IHOM measurement height of wind speed (height of anemometer) in meters

IBEWE time between two weather sequences in h,
 if LWOPT \neq 0, IBEWE is set to zero

 If LWOPT \neq 1 continue with S1

K1.3 Starting times of the weather sequences
 (FORMAT 8I10, as many cards as needed)

LWET(L) starting time of the weather sequences L in hours
 (L = 1,...LMAX)

 S1 If LPOPT \neq 1 continue with S2

K1.4 Probability distribution of the weather sequences
 (FORMAT 8E10.2, as many cards as needed)

PWET(L) probability of the weather sequences L;
 the sum over L must be 1 (L=1,...,LMAX)

 S2 For each site NS (NS = 1,...NSTMAX) the cards K1.5 to K1.7 are required.
 (not considered in UFOTRI, COSYMA relevant)

K1.5 Card of the site NS
 (FORMAT I2, A8, I10, 1PE10.2)

NRST number of identification of the site
 according to the population data file

STONAM(NS) name of the site

NSTOPT(NS) option for specifying the population data
 = 0 uniform population distribution POPDIC
 = 1 population distribution is defined by
 K1.7 for all distance bands
 = 2 population distribution is defined by
 K1.7 for the distance bands 1 to IEIN;
 outside it is uniform
 = 3 population distribution is defined by
 the site data file (NUNITS(31))

PSTO(NS) probability of the site; in general:
 PSTO = number of reactor blocks at the site/
 number of reactor blocks in the zone
 the sum over NS must be equal 1

 If NSTOPT(NS) = 1 continue with S3
 If NSTOPT(NS) = 3 continue with S4

K1.6 Card of the uniform population distribution
 (FORMAT E10.2, I10)

POPDIC uniform population density in people/km²

 IEIN index of the distance band up to which the
 population distribution is read from K1.7
 (only required if NSTOPT(NS) = 2).

 S3 For each angular segment J (J = 1,...JMAX) K1.7 is required.

K1.7 Card of the population distribution
 (FORMAT 8I10, as many cards as needed)

IPOP(J,I) population in each distance band I (I = 1,...,IMAX)
 for the angular segment J (see input group POLGRID).
 The middle of the first segment (J = 1) is 0 degree
 (order of the segments clockwise)

 S4 End of input group METEOZON

7.2.2 Input group SOURCE

This input group defines the release and its phases. Data relating to the start and duration of the release and reactor building dimensions have to be entered in strict column format.

K2.1 title card SOURCE
(FORMAT A8)

SOURCE name of identification (left-justified)

K2.2 Card of the source term
(FORMAT A8, 2X, 2I10)

UNFNAM name of the source term

NPHMAX number of release phases (max. NPHSMX)

IPZ shift of the beginning of all weather sequences
relative to the chosen starting times

For each release phase NP (NP=1,...,NPHMAX) K2.3 (and resp. K2.4) are required.

K2.3 Card of the release parameters for phase NP
(FORMAT 2I10, 3E10.3)

IPHASE(NP) time in whole hours between the end of the chain
reactions and the start of each release phase

IHO(NP) height of the release in meters

QH(NP) thermal energy of the release in cal/sec

BR(NP) width of the reactor building in meters

HOE(NP) height of the reactor building in meters

S5 End of input group SOURCE

7.2.3 Input group END

The input group END consists only of the card K3.1 and shows the end of the input data. If there is no mistake, the following message appears:

"END OF INPUT WITHOUT ERRORS"

K3.1 title card END
(FORMAT A8)

END name of identification (left-justified)

7.3 Optional input groups

7.3.1 Input group PRINTOUT

It is up to the user to define the amount of paper output to be produced (results and control output of input data) for general control parameters. The output shows mainly results from the primary dispersion model. Control output for tritium specific parameter and arrays will be defined in the tritium specific NAMELIST TRIDAT. The line printer output is assigned to unit NAUS (=6) for the control output of module INDAT and to unit NUNITS(6) (=6) for the result output. Even with the output set at a minimum, the amount of output is still quite large.

To get paper output of single values (i.e. all grid points for one weather sequence), the parameters named NOO... should be used. If they are set to 1, results are printed for ALL weather sequences. A value of 2 prints the results of the weather sequences selected by LKZ. LKZ is the index of the weather sequences that you can choose to be shown as output. It allows up to 20 to be chosen, but when choosing fewer, the remaining LKZ must be set to zero, e.g. if there are 30 weather sequences, in order to choose numbers 4, 7 and 23, LKZ = 4,7,23,17*0. IACT will show output of radii dependent results so the number of IACT equals IMAX. If R = 1000, 3500, 7500, and RA = 2000, 5000, 10000, to show results out to 2km, IACT = 1,2*0.

The title card of PRINTOUT is followed by the NAMELIST OUTPAR.

K5.1 title card PRINTOUT
(FORMAT A8)

PRINTOUT name of identification (left-justified)

K5.2 DATA CARD (NAMELIST-FORMAT)
NAMELIST OUTPAR

NAME	DEFAULT	DESCRIPTION
----	-----	-----
IBVOUT	1	option for printout of the population distribution ≠ 0 : printout for all sites = 0 : no printout

NOOTMT	0	option for printout of information about meteorological and trajectory data ≤ 0 no printout = 1 printout for all weather sequences = 2 printout for the weather sequences defined by LKZ
NOOTKZ	0	option for printout of concentrations for the radii defined by IACT, each sector and the nuclide group INUKL ≤ 0 no printout = 1 printout for all weather sequences = 2 printout for the weather sequences defined by LKZ
LKZ(L1) (20 values)	1,7,50, 75,90, 115, 14*0	gives the index of the weather sequences, for which a printout of nuclide concentrations is wanted (if less than 20 weather sequences are chosen, the remaining indices must be set to zero)
IACT(I) (20 values)	20*1	specifies whether a printout of radii dependent results is wanted for the distance band I = 0 no printout for distance I ≠ 0 printout for distance I

7.3.2 Input group POLGRID

In the input group POLGRID the user defines the grid for the population, agricultural production and land-sea distribution data and for the calculations of concentrations and individual doses and risks. It must precede the input group METEOZON. The title card is followed by the NAMELIST GRDPAR.

The grid consists of a polar coordinate system with the centre point at the location of the nuclear facility. The concentrations and individual doses and risks are calculated for a grid point representing the whole grid element. If you change the default values, you have to be sure to create new distance bands which are nearly representative for a square, in the view of the modelling of the re-emission part (see also physical description part UFOTRI /24/).

IMAX and JMAX are the number of radii and sectors respectively. RA is the outer radius of each radial band. IMAX, JMAX and RA must be identical to the parameters chosen when calculating the polar population distribution around the site. R is the reference point in the grid element chosen to represent the element as a whole, e.g. it could be halfway between two values of RA. UFOTRI refers to each distance band by its referenced point (centre), e.g. if RA=2000, 5000, 10000 and R=1000, 3500 and 7500, then doses for example given at 3500 m would be representative of the doses in the band from 2 to 5 km.

K6.1 title card POLGRID
(FORMAT A8)

POLGRID name of identification (left-justified)

K6.2 DATA CARD (NAMELIST-FORMAT)
NAMELIST GRDPAR

NAME	DEFAULT	DESCRIPTION
----	-----	-----
IMAX	20	number of radial distances (max. NRMAX)
JMAX	72	number of angular segments (max. NPHIMX)
R(I) (20 values)		radial grid; distance of the radii R(I), (I = 1,...,IMAX) in meters, completed with dummy values to NRMAX values
	65., 100., 145., 210., 320., 460., 680., 1000., 1500., 2100., 3200., 4600., 6800., 10000., 15000., 21000., 32000., 46000., 68000., 100000.	

RA(I) outer radius of the distance bands I
(20 values) (I = 1,...,IMAX) in meters, completed with

dummy values to NRMAL values

80., 120., 170., 260., 390.,
570., 840., 1250., 1750., 2600.,
3900., 5700., 8400., 12500., 17500.,
26000., 39000., 57000., 84000., 125000.

The values of the radii RA(I) and the angular segments must be identical with those used in the preprocessing program GRIDS (not included in this UFOTRI package) to calculate the population distribution.

7.3.3 Input group ISOTOPE

In the input group ISOTOPE the user has to define the physical characteristics of the NTYPMX nuclide groups NN. The sequence of the nuclides is **obligatory**

- 1. nuclide HT
- 2. nuclide HTO

The title card is followed by the NAMELIST ISOPAR.

K7.1 title card ISOTOPE
(FORMAT A8)

ISOTOPE name of identification (left-justified)

K7.2 DATA CARD (NAMELIST-FORMAT)
NAMELIST ISOPAR

NAME ----	DEFAULT -----	DESCRIPTION -----
NABL	2	number of type of nuclides with different deposition characteristics (max. NTYPMX) NOTE had to be set to 2 NOTE: sequence is obligatory (HT before HTO)
CORRVA(NN) (2 values)	2*1.0	correction factor for deposition velocity
VA(NN) (2 values)	0.0005 0.005	deposition velocity in m/sec for the nuclide group NN; NOTE: sequence is obligatory - NN = 1: HT-gas - NN = 2: HTO-vapour
IWASH	0	option for calculation of washout coefficient IWASH = 0: the washout coefficients and the mean relative duration of precipitation are precalculated for the nuclide groups NN and the precipitation intensity class IR IWASH = 1: the washout coefficients will be calculated according to the power law $XLAM(NN) = AWASH(NN) * (I^{**}BWASH(NN))$ for the nuclide groups NN, where I denotes the precipitation intensity in mm/h; a relative duration of rainfall can also be chosen,

If IWASH = 0 the following variables will be used:

IREGGR(IR1) (2 values)	100,300	boundaries of the rain intensity classes IR in 0.01 mm/h - IR = 1: rain intensity IREGGR(1) - IR = 2: rain intensity between IREGGR(1) and IREGGR(2) - IR = 3: rain intensity \geq IREGGR(2)
AMDA(NN,IR) (6 values)		washout coefficient in 1/sec for the rain intensity class IR and the nuclide group NN for IR = 1: 0.,0.00006, for IR = 2: 0.,0.00010, for IR = 3: 0.,0.00040,
REGTIM(NN,IR) (6 values)		mean duration of precipitation for the rain class IR and the nuclide group NN for IR = 1: 0., 0.5 for IR = 2: 0., 0.75 for IR = 3: 0., 0.72

If IWASH = 1 the following variables will be used:

AWASH(NN) (2 values)	0.0, 9.E-5	coefficient in power law for calculation of washout coefficient;
BWASH(NN) (2 values)	0.0, 0.6,	exponent in power law for calculation of washout coefficient, dependent on the nuclide group NN
REGTIM(NN,1) (2 values)	see above	mean duration of precipitation for the nuclide group NN, independent of any precipitation intensity class

7.3.4 Input group METEOROL

The input group METEOROL defines the parameters for the atmospheric dispersion part of UFOTRI. If desired (METIN \neq 0) the user can supply weather conditions for a single weather sequence with straight-line Gaussian modelling consisting of one phase. The title card is followed by the NAMELIST METPAR.

K8.1 title card METEOROL
(FORMAT A8)

METEOROL name of identification (left-justified)

K8.2 DATA CARD (NAMELIST-FORMAT)
NAMELIST METPAR

NAME ----	DEFAULT -----	DESCRIPTION -----
METIN	0	0: Option to read the meteorological data from file with changing weather conditions. \neq 0: Option to start one single straight-line Gaussian calculation without changing weather. The data of the atmospheric dispersion and deposition parameters are supplied by the user in the NAMELIST METPAR (IWDR, IWDRG, IDIKAT, IREGN and MIXLH must be given there; additional parameters had to be set in the NAMELIST TRIDAT, see later on)
NOSHFT	2	option for the treatment of changes in wind direction during dispersion: = 0 straight-line dispersion model; all release phases are transported in the same direction = 1 straight-line dispersion; each release phase is transported in the direction of the wind at its beginning = 2 for each release phase hourly changes in wind direction are considered
IWDR	360	wind direction in degrees
IWDRG	500	wind speed in 1/100 m/sec
IDIKAT	4	diffusion category (1 through 6, representing the categories A through F)
IREGN	0	rain rate in 1/100 mm/h
HGHT(IH) (IH=1,3)	50.,100.,180.	height for the σ -parameters in meters
MIXLH(ISK) (ISK=1,6)	1600,1200,800, 560, 320,200	height of the mixing layer in meters for each diffusion category ISK; (ISK = 1,...,6 represents the diffusion categories A through F)

WPE(ISK)	0.07,0.13,	wind profile exponent for the diffusion
(ISK=1,6)	0.21,0.34,	categories ISK (ISK = 1,...,6 represents the
	0.44,0.44	categories A through F)

The horizontal and vertical dispersion parameters are calculated as a function of distance x assuming the following power law (see KfK-4332)

$$\sigma_y = PY1 \cdot x^{QY1}$$

$$\sigma_z = PZ1 \cdot x^{QZ1}$$

The downwind diffusion is modelled in UFOTRI by the dispersion parameter σ_x ; as long as $\sigma_x < \sigma_y$, it is calculated due to

$$\sigma_x = \frac{2}{3} x \tan STETA1;$$

for $\sigma_x \geq \sigma_y$, it is assumed that $\sigma_x = \sigma_y$ (see KfK-4332, p. 15 - 17).

PZ1(ISK, IH, IRH)	linear term of the formula to calculate σ_z for:
(6*3*2 values)	- 6 diffusion categories ISK
	- 3 classes of height IH
	- 2 classes of roughness IRH
	(IRH = 1 : roughness IRAU = 2
	IRH = 2 : roughness IRAU = 3)
	1.321,0.950,0.700,0.520,0.382,0.311,
	1.321,0.950,0.700,0.520,0.382,0.311,
	1.321,0.950,0.700,0.520,0.382,0.311,
	0.151,0.127,0.165,0.215,0.264,0.241,
	0.051,0.070,0.137,0.265,0.487,0.717,
	0.025,0.033,0.104,0.307,0.546,0.485

QZ1(ISK, IH, IRH)	exponential term of the formula to calculate σ_z for:
(6*3*2 values)	- 6 diffusion categories ISK
	- 3 classes of height IH
	- 2 classes of roughness IRH
	(IRH = 1 : roughness IRAU = 2
	IRH = 2 : roughness IRAU = 3)
	6*0.711,6*0.711,6*0.711,
	1.219,1.108,0.996,0.885,0.774,0.662,
	1.317,1.151,0.985,0.818,0.652,0.486,
	1.500,1.320,0.997,0.734,0.557,0.500

PY1(ISK, IH, IRH)	linear term of the formula to calculate σ_y for:
(6*3*2 values)	- 6 diffusion categories ISK
	- 3 classes of height IH
	- 2 classes of roughness IRH
	(IRH = 1 : roughness IRAU = 2
	IRH = 2 : roughness IRAU = 3)
	0.946,0.826,0.586,0.418,0.297,0.235,
	0.946,0.826,0.586,0.418,0.297,0.235,
	0.946,0.826,0.586,0.418,0.297,0.235,

1.503,0.876,0.659,0.640,0.801,1.294,
 0.170,0.324,0.466,0.504,0.411,0.253,
 0.671,0.415,0.232,0.208,0.345,0.671

QY1(ISK,IH,IRH) exponential term of the formula to calculate σ_y for:
 (6*3*2 values) - 6 diffusion categories ISK
 - 3 classes of height IH
 - 2 classes of roughness IRH
 (IRH = 1 : roughness IRAU = 2
 IRH = 2 : roughness IRAU = 3)

6*0.796,6*0.796,6*0.796,
 0.833,0.823,0.807,0.784,0.754,0.718,
 1.296,1.025,0.866,0.818,0.882,1.057,
 0.903,0.903,0.903,0.903,0.903,0.903

STETA1(ISK,IH,IRH) horizontal standard-deviation (in degree) of wind
 (6*3*2 values) direction for:
 - 6 diffusion categories ISK
 - 3 classes of height IH
 - 2 classes of roughness IRH
 (IRH = 1 : roughness IRAU = 2
 IRH = 2 : roughness IRAU = 3)

20.5,13.9,10.1,6.9,4.,2.,
 20.5,13.9,10.1,6.9,4.,2.,
 20.5,13.9,10.1,6.9,4.,2.,
 23.8,18.9,15.3,12.6,10.2,8.6,
 20.5,13.9,10.1,6.9,4.,2.,
 20.5,13.9,10.1,6.9,4.,2.

7.4 Parameters controlling the model part with an hourly timestep for atmospheric dispersion and the longer term ingestion pathways

The input parameters which are listed in this chapter belong to one single input group called 'TRIDAT'.

7.4.1 General control parameters

In this part of the input group TRIDAT general control parameters will be specified. Of special interest for the user may be four parameters which will be described in the following.

Q determines the relative amount of each of both chemical forms HT and HTO of the source term and Q1 contains the absolute amount of the source term in Bq per timestep and phase. BODFAK determines the minimum source strength of a secondary area source of HTO from the soil and the vegetation, which will be considered in the re-emission dispersion part. The minimal source strength will be calculated as

$$\text{minimal source strength} = \text{maximal soil concentration} \times \text{BODFAK}$$

The smaller the minimal source strength, the more computing time will be needed. The below listed values for BODFAK are useful:

BODFAK	release case
1	HT-release
100	HTO-release
10	HTO-release with building wake effects
0.1	HT-release with building wake effects

The fourth important parameter NSTOP controls the minimal duration of the atmospheric dispersion part with its more accurate modelling of all transfer processes. But the greater NSTOP is, the more computing time will be needed, however the results will be more defensible. Test calculations with the model have shown, that values of NSTOP greater than 170 hours give no significant changes in the resulting dose, because the dispersion of tritium due to atmospheric processes are no longer important.

BODFAK = A factor which will be multiplied by the maximum air concentration for defining the minimum source strength of an area source which will be considered in the re-emission dispersion part
(DEFAULT = 100.)

- NSTOP** = Minimal duration of the re-emission process in hours; the re-emission program stops after **NSTOP** hours and the amount of activity in the soil is reduced to the third part of the tritium content after the re-emission routine has started
(DEFAULT = 70)
- IZFREI** = Duration of the release of the primary plume in seconds; is only important for line printer output of concentrations in air
 $0 < \text{IZFREI} < 3600$
(DEFAULT = 3600)
- IFLENG** = Flag to define the area source geometry for the re-emission algorithm
= 1 narrow area source with 6 grid points
Notice if the narrow area source geometry is selected, a special radial grid has to be considered, which is different from the normally used one
= 0 normal area source with 14 grid points
(DEFAULT = 0)
- Q(NN,J)** = Relative source strength of the nuclide type NN in the phase J
 $0. \leq Q \leq 1.$
(DEFAULT = 17 * 0., 17 * 1.)
- Q1(J)** = Absolute source strength in the phase J
(DEFAULT = 17 * 1.)
- ARAU** = Roughness length in m
(DEFAULT = 0.3)
- ZEIT** = Time interval between meteorological recordings
NOTE had to be 3600.
(DEFAULT = 3600.)
- CHIMAX** = Minimum value of the time integrated air concentration (cut-off value in Bq s / m³; used also for ingestion module)
(DEFAULT = 1.E-15)
- NUKL(NN)** = names of chemical forms of tritium considered in UFOTRI
(DEFAULT NN = 1 : 'HT '
NN = 2 : 'HTO ')
- NJAHRE** = Number of years with meteorological data
 $\text{NJAHRE} \geq 1$
(DEFAULT = 1)
- LT1** = First day of the vegetation period for the first year

(DEFAULT = 90)

- LT2** = Last day of the vegetation period for the first year
(DEFAULT = 303)
- LT3** = First day of the vegetation period for the second year
(DEFAULT = 455)
- LT4** = Last day of the vegetation period for the second year
(DEFAULT = 670)

7.4.2 Special submodels used in UFOTRI

Within the UFOTRI code the possibility is offered to use submodels of different complexity for calculating the deposition velocity of HT/HTO (IDEPHT, IFLAGS with IFLAGR), the evapotranspiration (IMODEL, IMONT, IFLAGR), the water movement in soil (IBODEX) and the conversion rates from HTO to OBT (ICOVER, IPHOTO, IMODEL). The advanced models are mainly based on resistance approaches.

- IMODEL** = Choice of the model for calculating the plant resistance
 = 1 extended model will be used considering:
 radiation balance, air temperature, air humidity, water content of soil,
 water stress from high solar radiation
 = 0 simple model will be used considering:
 day/night cycle, water content of soil, water stress from high solar radiation
 (DEFAULT = 1)
- ICOVER** = Choice of the model for calculating the actual plant stage
 = 1 replacing the initial values by the calculated ones
 = 0 initial values used
 (DEFAULT = 1)
- IPHOTO** = Choice of the model for calculating the transfer HTO-OBT fruits
 = 1 calculating the photosynthesis rate which is associated with the
 hourly transfer rates into OBT
 = 0 diurnal transfer rates are used
 (DEFAULT = 1)
- IMONT** = Choice of the model for calculating the evapotranspiration
 = 1 Monteith resistance approach is applied
 = 0 Penman formula is used
 (DEFAULT = 1)
- IFLAGS** = Switch for the calculation of the HTO deposition velocity to soil
 = 1 uses the resistance model
 = 0 uses the predefined deposition velocity
 (DEFAULT = 1)
- IFLAGR** = Switch for the calculation of the soil resistance, (only if IFLAGS = 1)
 = 1 uses the resistance model
 = 0 uses the predefined soil resistance value (RSOIL = 150 s/m)
 (DEFAULT = 1)
- IDEPHT** = Switch for the calculation of the HT deposition velocity to soil

- = 1 uses the resistance model
 - = 0 uses the predefined deposition velocity
- (DEFAULT = 1)

- IBODEX** = Choice of the model for calculation of the water transport in soil
- = 1 extended model will be used with the calculation of the suction tension and soil conductivity:
 - formula for suction tension:
$$SS = 1.5E5 * PSI1^{**}(AP + BP*PSI1 + CP*PSI1^{**}NP)$$
 - formula for conductivity:
$$COND = AKP / (SS^{**}MKP + BKP)$$
 - = 0 simple model will be used
- (DEFAULT = 1)

7.4.3 Plant parameters

In this part of the input group TRIDAT four different plant specific parameter sets will be defined. Two parameters for the plant body and two additional ones for the edible parts, (BEW###), determine the fraction of organic and anorganic matter content of the vegetation for every plant species. At least two parameters (RCMIN#, LEAF##) are necessary to calculate the stomata resistance which is needed for calculation of the exchange plant-atmosphere (model of Belot). If the extended model for calculating the stomata resistance is recommended (IMODEL = 1), five additional parameters (RCPAR#, VDP#, TMIN#, TMAX#, TOPT#) have to be defined. Two parameters (DISSOZ and CO2DRY) are necessary for the photosynthesis model. ISTRGR is a plant independent parameter indicating the occurrence of stomata closure due to high solar insolation.

- ISTRGR** = If the solar radiation has greater values than ISTRGR, water stress will occur. **Note** the dimension is $\text{Watt/m}^2 \times 0.357 \times 0.8$
(DEFAULT = 200)
- RCMIN** = Minimal stomata diffusion resistance normalized to a leaf area index of 1, **for area 1**
(DEFAULT = 2.0)
- BEWG** = Weight of vegetation water in g / m^2 **for area 1**
(DEFAULT = 1440.0)
- BEWGZ** = Mass content of the organic parts of the plant in g / m^2 **for area 1**
(DEFAULT = 160.0)
- LEAF** = Leaf area index in m^2 / m^2 **for area 1**
(DEFAULT = 3.0)
- RCPARA** = Constant equal to the photosynthetic radiation flux density measured at a stomata resistance two times higher than the minimum value **for area 1; if IMODEL = 1**
(DEFAULT = 20.0)
- VPDA** = Constant related to the vapour pressure deficit **for area 1; if IMODEL = 1**
(DEFAULT = 0.2)
- TMINA** = Minimum temperature at which stomata closure occurs in $^{\circ}\text{C}$ **for area 1; if IMODEL = 1**
(DEFAULT = 0.0)

- TMAXA** = Maximum temperature at which stomata closure occurs in °C for area 1;
(DEFAULT = 45.0)
- TOPTA** = Optimum temperature for photosynthesis in °C for area 1;
if **IMODEL = 1**
(DEFAULT = 25.0)
- RCMIN2** = Minimal stomata diffusion resistance normalized to a leaf area index of 1, for area 2
(DEFAULT = 2.0)
- BEWG2** = Weight of vegetation water in g / m² for area 2
(DEFAULT = 680.0)
- BEWGZ2** = Mass content of the organic parts of the plant in g / m² for area 2
(DEFAULT = 170.0)
- LEAF2** = Leaf area index in m² / m² for area 2
(DEFAULT = 3.0)
- RCPARG** = Constant equal to the photosynthetic radiation flux density measured at a stomata resistance two times higher than the minimum value for area 2; if **IMODEL = 1**
(DEFAULT = 20.0)
- VPDG** = Constant related to the vapour pressure deficit for area 2;
if **IMODEL = 1**
(DEFAULT = 0.2)
- TMING** = Minimum temperature at which stomata closure occurs in °C for area 2; if **IMODEL = 1**
(DEFAULT = 0.0)
- TMAXG** = Maximum temperature at which stomata closure occurs in °C for area 2; if **IMODEL = 1**
(DEFAULT = 45.0)
- TOPTG** = Optimum temperature for photosynthesis in °C for area 2;
if **IMODEL = 1**
(DEFAULT = 25.0)
- RCMINP** = Minimal stomata diffusion resistance normalized to a leaf area index of 1, for potatoes
(DEFAULT = 1.5)
- BEWGP** = Weight of vegetation water in g / m² for potatoes

- (DEFAULT = 2400.0)
- BEWGZP** = Mass content of the organic parts of the plant in g / m² **for potatoes**
(DEFAULT = 600.0)
- BEWGPR** = Weight of water of bulbs in g / m² **for potatoes**
(DEFAULT = 2340.0)
- BEWZPR** = Mass content of the organic parts of the bulbs in g / m² **for potatoes**
(DEFAULT = 660.0)
- LEAFP** = Leaf area index in m² / m² **for potatoes**
(DEFAULT = 4.7)
- RCPARP** = Constant equal to the photosynthetic radiation flux density measured at a stomata resistance two times higher than the minimum value **for potatoes; if IMODEL = 1**
(DEFAULT = 50.0)
- VPDP** = Constant related to the vapour pressure deficit **for potatoes; if IMODEL = 1**
(DEFAULT = 0.2)
- TMINP** = Minimum temperature at which stomata closure occurs in °C **for potatoes; if IMODEL = 1**
(DEFAULT = 0.0)
- TMAXP** = Maximum temperature at which stomata closure occurs in °C **for potatoes; if IMODEL = 1**
(DEFAULT = 45.0)
- TOPTP** = Optimum temperature for photosynthesis in °C **for potatoes; if IMODEL = 1**
(DEFAULT = 25.0)
- RCMINW** = Minimal stomata diffusion resistance normalized to a leaf area index of 1, **for wheat**
(DEFAULT = 2.0)
- BEGWG** = Weight of vegetation water in g / m² **for wheat**
(DEFAULT = 2000.0)
- BEWGZW** = Mass content of the organic parts of the plant in g / m² **for wheat**
(DEFAULT = 500.0)
- BEGWWR** = Weight of water in the cereals in g / m² **for wheat**
(DEFAULT = 81.0)

- BEWZWR** = Mass content of the organic parts of the cereals in g / m² **for wheat**
(DEFAULT = 519.0)
- LEAFW** = Leaf area index in m² / m² **for wheat**
(DEFAULT = 7.0)
- RCPARW** = Constant equal to the photosynthetical radiation flux density measured
at a stomata resistance two times higher than the minimum value **for**
wheat; if IMODEL = 1
(DEFAULT = 30.0)
- VPDW** = Constant related to the vapour pressure deficit **for wheat;**
if IMODEL = 1
(DEFAULT = 0.2)
- TMINW** = Minimum temperature at which stomata closure occurs in °C **for wheat;**
if IMODEL = 1
(DEFAULT = 0.0)
- TMAXW** = Maximum temperature at which stomata closure occurs in °C **for wheat;**
if IMODEL = 1
(DEFAULT = 45.0)
- TOPTW** = Optimum temperature for photosynthesis in °C **for wheat;**
if IMODEL = 1
(DEFAULT = 25.0)
- CO2DRY** = Conversion factor CO₂ to dry matter, necessary **if IPHOTO = 1**
(DEFAULT = 1.5)
- DISSOZ** = Multiplication factor (normally < 1) taking into account for the nonuni-
form tritium distribution in plants (photosynthesis relevant parts); ne-
cessary for tranfer HTO to OBT **if IPHOTO = 1**
(DEFAULT = 0.5)

7.4.4 Soil parameters

The following parameters describe mainly the characteristics of the soil properties and the procedure how the initial water content is used as input. Additionally, some special re-emission conditions such as re-emission rate of the soil during the night-time and during rain events and the overall change of re-emission rate can be influenced by REMRE, REMNI, REDREM, respectively.

A very important parameter which occurs in this part is BODEIN, the initial water content of the soil (equal for all four areas). Test calculations demonstrated that the collective and individual dose from the ingestion pathways react sensitive to changes of BODEIN, especially near the wilting point. Therefore a switch (IBODFX) is introduced to decide if the initial water content is taken from a file or not. If not, the BODEIN represents the initial water content of all weather sequences of one model run (they are all equal). If yes, the initial water content of the soil has to be precalculated by a hydrological model for each hour of the meteorological dataset. The value of the starting hour will be taken as the initial soil water content. The precalculated soil moisture is part of the meteorological input file, which is described in detail in chapter 5.

The extended soil transport model (IBODEX = 1) describes water transfer between the soil layers due to matrix forces.

- IBODFX** = Switch for the initial water content (3 layers)
 = 1 reads the value from file (precalculated)
 = 0 uses the predefined BODEIN value (equal for all 3 layers)
 (DEFAULT = 0)
- BODEIN** = Initial value of the fraction of the soil water content
 0.2 means 20% water content in the soil; maximum is SOILMX*100%
 (DEFAULT = 0.2)
- SOILMX** = Fraction of the maximum free pore volume of soil
 (DEFAULT = 0.5)
- WILTP** = Wilting point, stomata closure occurs
 (DEFAULT = 0.1)
- IARTBO** = Only valid if IBODEX = 1; selects the soil characteristics
 = 1 humus sandy loam; (special default values used)
 = 2 loamy sand; (special default values used)
 = 3 sand; (special default values used)
 = 4 the user may define his own soil type with the following 7 parameters
 for calculating the suction tension and soil conductivity:
 formula for suction tension:

$$SS = 1.5E5 * PSI1^{**}(AP + BP*PSI1 + CP*PSI1^{**}NP)$$

formula for conductivity:

$$\text{COND} = \text{AKP} / (\text{SS}^{**}\text{MKP} + \text{BKP})$$

(DEFAULT = 1)

- SOILAP** = Parameter for calculating the suction tension: AP
(DEFAULT = 1.65)
- SOILBP** = Parameter for calculating the suction tension: BP
(DEFAULT = 7.3)
- SOILCP** = Parameter for calculating the suction tension: CP
(DEFAULT = -3.1)
- SOILNP** = Parameter for calculating the suction tension: NP
(DEFAULT = 7.5)
- SOIAKP** = Parameter for calculating the conductivity: AKP
(DEFAULT = 1000.)
- SOIBKP** = Parameter for calculating the conductivity: BKP
(DEFAULT = 60.0)
- SOIMKP** = Parameter for calculating the conductivity: MKP
(DEFAULT = 1.41)
- RSOIL** = Soil resistance in s/m (necessary if **IFLAGS = 1**, **IFLAGR = 0** => simple resistance model with constant value has been switched on)
(DEFAULT = 150.)
- RSSMIN** = Minimum soil resistance in s/m (necessary if **IFLAGS = 1**, **IFLAGR = 1** => resistance model has been switched on)
(DEFAULT = 50.)
- ZSOILA** = Initial resistance depth of soil in m (necessary if **IFLAGS = 1**, **IFLAGR = 1** => resistance model has been switched on)
(DEFAULT = 0.004)
- REMRE** = Re-emission rate during rain events in % per hour
(DEFAULT = 0.3)
- REMNI** = Re-emission rate during the night in % per hour
(DEFAULT = 1.0)
- REDREM** = Factor varying the re-emission rate
(DEFAULT = 1.0)

7.4.5 Parameters for the short term ingestion pathways

The parameters listed below determine the fractions of the agricultural used land areas, the pasture land areas, areas for potato and winter wheat production, respectively (FAKC1, FAKC2, FAFCP, FAKCW). Five parameters (NCOW to NASS) control the water balance of the atmosphere, the number of cows which are grazing on one square kilometre and the organic and anorganic matter content of the cows. The parameters IRELIN, IHARP, IHARW define the day of release, the day of harvesting for potatoes and winter wheat, respectively.

FAKC1	=	Fraction of the area reserved for agricultural production and vegetation Note: sum of all areas = 1 (DEFAULT = 0.4)
FAKC2	=	Fraction of the area reserved for grazing animals Note: sum of all areas = 1 (DEFAULT = 0.2)
FAKCP	=	Fraction of the area reserved for production of potatoes Note: sum of all areas = 1 (DEFAULT = 0.2)
FAKCW	=	Fraction of the area reserved for production of wheat Note: sum of all areas = 1 (DEFAULT = 0.2)
NCOW	=	Number of cows, grazing on one square kilometre (DEFAULT = 250)
WWCOW	=	Mass content of the anorganic part (water) of a cow in kg per cow (DEFAULT = 350.0)
WOCOW	=	Mass content of the organic fraction of a cow in kg per cow (DEFAULT = 150.0)
WATM	=	Mass of water in the atmosphere in kg / km ³ (DEFAULT = 8.0E + 6)
NASS	=	Mass of rain reaching the ground per day in kg / km ³ d (DEFAULT = 1.93E + 6)
IRELIN	=	Day of release (DEFAULT = 181)
IHARP	=	Day of harvest for potatoes

(DEFAULT = 258)

IHARW = Day of harvest for wheat
(DEFAULT = 225)

7.4.6 Parameters for the food restriction module

UFOTRI allows for the calculation of food restrictions. Therefore, the intervention level for food banning (COGRF) and the intervention times (= days after the release for calculation of concentrations) have to be assigned a value. The TIMEDO values overwrite the TIMC values used in the previous version of UFOTRI. The first 2 values of TIMEDO are of importance only for the inhalation dose and should be 1 and 3, but internally UFOTRI will overwrite these values which will be set to 24 and 72 hours. However, the time dependent doses from inhalation are only of importance if UFOTRI is coupled with COSYMA. One time value within the TIMEDO array has to be greater than 365 (better > 1000). This is the endpoint for the integration time of the dose module for all the continuously harvested foodstuffs (meat, milk and vegetables). The foodstuffs with a fixed harvesting time will be consumed for one year only independent of the high value in the TIMEDO array.

Note that the effective dose equivalent which is stored for further evaluation will not be affected by the food restriction module. The doses calculated herein will be stored separately on the logical unit 95, if IBANWR is set to 1.

FOODST(5) = Name of foodstuff
(DEFAULT = meat, milk, vegetables, potatoes, wheat; character * 10)

COGRF(5) = Intervention level for food restriction in Bq / kg fresh weight (for 5 foodstuffs)
(DEFAULT = 5 * 1250)

TIMEDO(12) = Time after release for check of application or removing of food restrictions (days)
(DEFAULT = 1,3,7,14,21,30,90,180,200,360,2*3600)

ITIMD = Flag for printout on paper of doses and concentrations for time TIMEDO(ITIMD)
(DEFAULT = 20, no printout)

IBANWR = switch for storage
= 0 no storage
= 1 storage on the logical UNIT 95
(DEFAULT = 0)

7.4.7 Long term ingestion pathways

The parameters presented here are necessary for the calculation of the longer term behaviour of tritium in the environment. They control the compartment module which runs after the dispersion and re-emission model. The most important point is that NBOX, NINI, NINT and NOUT have to be set to the same values. Allowed is in principle only the value 10. The value 6 from the former program version is not tested and may result in errors.

The variables NTIM and TIMC from the former UFOTRI version has been dropt off. The meaning has been shifted to the TIMEDO and ITIMD variables, defined within the food restriction part.

NBOX	=	Number of compartments (10 for both areas and 6 for agricultural areas only) (DEFAULT = 10)
NINI	=	Number of compartments with an initial inventory = NBOX (10 for both areas and 6 for agricultural areas only) (DEFAULT = 10)
NINT	=	Number of integrals with an initial inventory = NBOX (10 for both areas and 6 for agricultural areas only) (DEFAULT = 10)
NOUT	=	Number of inventories = NBOX (10 for both areas and 6 for agricultural areas only) (DEFAULT = 10)
NTFX	=	Number of transfer coefficients (27 should not be changed, will be rearranged in the program dependent on summer or winter) (DEFAULT = 27)

7.4.8 Parameters for dose calculations

The parameters in the equations for the dose calculations consist of two groups. Three parameters contain values for the dose conversion factor, dependent on the age of the individual and the integration time, whereas other parameters determine the breathing rate, the rate of uptake through the skin and the ingestion habits of the population group of interest. However, for a standard run an adult and the 50 year committed effective dose equivalent (EDE) are recommended.

BRRATE	=	Breathing rate of an individual in m^3 / s (DEFAULT = $3.3\text{E-}4$)
SKRATE	=	Rate of skin uptake of an individual in m^3 / s (DEFAULT = $1.4\text{E-}4$)
IMEAT	=	Consumption rate of meat for an individual in gram per day (DEFAULT = 206)
IVEGE	=	Consumption rate of vegetables for an individual in gram per day (DEFAULT = 165)
IMILK	=	Consumption rate of milk products for an individual in gram per day (DEFAULT = 315)
IPOT	=	Consumption rate of potatoes for an individual in gram per day (DEFAULT = 192)
IWHEAT	=	Consumption rate of wheat for an individual in gram per day (DEFAULT = 261)
DOSF	=	EDE-Dose conversion factor in Sv/Bq (HTO) for an individual (DEFAULT = $1.7\text{E-}11$)
DOSHT	=	EDE-Dose conversion factor in Sv/Bq (HT) for an individual (DEFAULT = $1.7\text{E-}15$)
DOSFOB	=	EDE-Dose conversion factor in Sv/Bq (OBT) for an individual (DEFAULT = $4.0\text{E-}11$)

7.4.9 Parameters controlling a fixed stationary run

If the user selects a run with fixed meteorology (METIN = 1 in the input group METEOROL) the both remaining input parameters temperature and solar insolation have to be set to fixed values, too. Additionally a fixed re-emission rate of HTO from the soil and the plants may be chosen. A fixed exchange rate plant-atmosphere can hardly be defined, because of the strong implications and the dynamic interactions of all processes concerning the vegetation. However there exists a second possibility to have nearly stationary run conditions. If the environmental parameters remain constant, the model calculates implicitly a nearly constant exchange rate plant-atmosphere. Only the exchange soil to atmosphere will vary due to loss of water from the soil.

Note: only recommended for testing.

- IRFIX** = Flag to specify the re-emission rate
 = 1 fixed re-emission rate
Note: should be used carefully. It is a relict of the first stages of the development of the program. The fixed values of re-emission and plant deposition rate have to be changed in the program, if desired
 = 0 re-emission rate will be calculated by the program (normal mode)
 (DEFAULT = 0)
- REFEST** = Value of a fixed re-emission rate in % per hour
 (DEFAULT = 5.0)
- ITEMPE** = Fixed value for the air temperature during the whole run in °C × 100;
Note: will be considered if **METIN** is set to 1 (METIN belongs to another namelist called METPAR, input group METEOROL)
 (DEFAULT = 1000)
- ISTRBE** = Fixed value for the radiation balance during the whole run in Watt;
Note: will be considered if **METIN** is set to 1 (METIN belongs to another namelist called METPAR, input group METEOROL)
 (DEFAULT = 100)
- RELFA** = Fixed value for relative humidity in air in percent; **Note:** will be considered if **METIN** is set to 1 (METIN belongs to another namelist called METPAR, input group METEOROL)
 (DEFAULT = 0.5)

7.4.10 Parameters controlling input and output listings

The parameters listed above control the storage of results on permanent files as well as the output listing on line printer.

- IFACHS** = Index of the sector position in the polar grid system for printer control output
(DEFAULT = 28)
- IEINR#** = 4 values: IEINR1 - IEINR4
Index of the radius position in the polar grid system for printer control output
(DEFAULT = 6, 8, 12, 16)
- IZUAUS** = Flag steering additional control output during each time step on line printer (much lines consuming)
= 1 very much control output
= 0 no special control output
(DEFAULT = 0)
- KAUSDR(12)** = Array of 12 flags steering additional control output which will be printed on line printer (very much lines consuming)
= 1 control output
= 0 no control output
KAUSDR(1) - KAUSDR(3) controls output for the basic results
KAUSDR(4) controls output of subroutine which calculates the doses values
KAUSDR(5) controls output of subroutine which calculates possible food restrictions and areas affected by food restrictions
KAUSDR(7) controls output of subroutine which calculates the transfer factors
KAUSDR(8) controls output of subroutine which calculates the re-emission area and source strength
KAUSDR(9) controls output of subroutine which calculates the processes in the soil and in plants
KAUSDR(10) controls output of subroutine which calculates the dispersion process and environmental conditions of the re-emission process
KAUSDR(11) controls output of subroutine which calculates the dispersion process and environmental conditions of the re-emission process
KAUSDR(12) controls output of subroutine which calculates the long term ingestion doses
(DEFAULT = 12*0)

- IPRPLT** = Controls if a two dimensional printerplot of unit release concentrations is created for one chemical form of tritium (INUKL), but for each phase
- = 0 no printerplot
 - = 1 printerplot for all weather sequences
 - = 2 printerplot only for the weather sequences defined by LKZ (see e.g. PRINTOUT, namelist OUTPAR)
- (DEFAULT = 0)
- INUKL** = Index of the chemical form of tritium for which the concentrations are plotted by printerplot
- (DEFAULT = 2)
- IWRITE** = Controls if doses from inhalation + skin absorption and doses from the ingestion pathways are stored on the logical UNIT 9 for each weather sequence and each phase
- = 0 no storage
 - = 1 storage on the logical UNIT 9
- (DEFAULT = 0)
- LWETE** = For each weather sequence LW with $\text{MOD}(\text{LW}, \text{LWETE}) = 0$ a control printout will be created; should be used only for testing
- (DEFAULT = 1000)

8. Run the model

8.1 Introduction

At first it has to be pointed out, that UFOTRI needs some special subroutines from a mathematical library called **IMSL**. The long term ingestion model uses some of these subroutines for calculating the eigenvectors and eigenvalues of the matrix of the transfer rates (see Table 2 and 3). There exists several differing versions of the IMSL library. For two of them (IMSL-'old' and IMSL 11.1) exist a separate UFOTRI version. If the computer system does not include the IMSL library, another library with equivalent subroutines (NAG) in **double precision** mode has to be selected. Most of the program code is written in standard FORTRAN 77 except the NAMELIST (see chapter 6) and the INCLUDE statement.

The easiest way to gain experience is to start with the example calculation distributed with program package. Additionally, it is strongly recommended to read the basic main report of UFOTRI /24/ and the second chapter of this report, to get a better understanding of the possibilities of the code. Both reports describe the physical behaviour of tritium in the environment, as it is included in the present model version.

A list of the most important subroutines called within UFOTRI (Tab. 6 to Tab. 8) as well as 3 flow charts (Fig. 14 to Fig. 16) are attached to give the user a first understanding of UFOTRI.

8.2 Special input data-set for UFOTRI (meteorological file)

The meteorological data file contains information on the stability (Pasquill Turner categories), the wind direction, the wind speed, the precipitation intensity, the air temperature the relative humidity, the solar radiation balance and the water content in 3 soil layers. These data should be available for one meteorological observation station representative for the site with a temporal observation interval of one hour. The first data of the day contains the averaged values for the first hour (24:00 to 1:00). If no data for the water content in soil is available, dummy variables should be included in the meteorological file. Then the water content has to be defined within the NAMELIST TRIDAT (see parameter IBODFX and BODEIN). The data have to be available on a Direct Access File. One record of the file contains data for one day in the following order:

WR(J), IDIFF(J), IRAIN(J), WG(J), ITEMP(J), ISTRB(J), RELF(J), ISOIL1(J), ISOIL2(J), ISOIL3(J), J = 1,24

No. of variable	Variable	Type	length in byte b_i	meaning
1	WR	INT*4	4	Wind direction in °C
2	IDIFF	INT*4	4	Pasquill-Turner Stability class; conversion in (1=A, 2=B, 3=C, 4=D, 5=E, 6=F)
3	IRAIN	INT*4	4	Rain intensity in mm/h*100
4	WG	INT*4	4	Wind speed in meter * 100
5	ITEMP	INT*4	4	Air temperature in °C x 100
6	ISTRB	INT*4	4	Solar radiation in Watt / m**2
7	RELF	REAL*4	4	Relative humidity in % / 100.
8	ISOIL1	INT*4	4	Water content in soil 1 in % / 100.
9	ISOIL2	INT*4	4	Water content in soil 2 in % / 100.
10	ISOIL3	INT*4	4	Water content in soil 3 in % / 100.

In the current version the length of one record equals 960 byte (= $\sum_{i=1}^{10} b_i \times 24$).

Generally the meteorological input data file has the following characteristics :

ACCESS : DIRECT

RECL : $\sum_{i=1}^{10} b_i \times 24$

BLKSIZE : = RECL

RECFM : F = FIXED

The **whole** dataset contains **NDAYS** records, where

NDAYS = NYEARS * MAXDAY = max. number of days with met. data

The meteorological data have to be prepared unformatted and binary. They have to be available on logical input **unit 11**.

8.3 Output of UFOTRI

Output of UFOTRI are time dependent / time integrated concentrations and time dependent / effective dose values for:

- **temporal resolution:** for each phase and each weather sequence defined in the NAMELIST (one weather sequence may contain several release phases)
- **spatial resolution:** for the whole area under consideration and/or one special grid point.

The concentrations are in most cases specific ones, on the basis of wet or dry weight of a certain compartment (Bq/g and Bq/ml). Only the concentrations in air and on the soil surface (Bq/m³ and Bq/m²) have not been derived on a mass basis.

Two types of dose definitions will be used in UFOTRI

- The individual early dose from short-term exposure (only inhalation + skin absorption) and short-term integration
- The individual (collective) committed effective dose equivalent (EDE) from long-term exposure and 50 years integration time

The doses values stored on disk and/or printed on screen / paper are in general dose values from one release phase. Only results from the food restriction module will be stored and/or printed at the end of one weather sequence. These values have been accumulated for all phases.

In general one has to decide between storage on disc for further evaluation and printout on screen / paper.

- **Output on file** (see also Table 4)

unit 21: The output on the logical unit 21 for each weather sequence contains 3 different dose arrays. The dose values are by its default definition effective doses (EDE). But this may be changed by the user via the dose conversion factors. Doses will be calculated for inhalation + skin absorption resulting from plume passage only (first array). The second array contains the total dose from inhalation + skin absorption which includes also the whole re-emission period (+ long term module). The third array contains the chronic dose from the ingestion pathways

unit 91, 92, 93: For testing, some selected concentration (time course at a selected grid point during the reemission phase) and dose values will be stored permanently on disc. A description of the arrays can be found in the program.

unit 95: The time dependent dose values from the inhalation + skin absorption as well as the time dependent doses from ingestion with and without food restrictions will be stored on the disc with the logical unit 95.

- **Output on screen / paper**

unit 6: The EDE values, which will be stored on unit 21 can be printed on paper for each weather sequence. Additionally the array with the early dose (TIMEDO(3) days exposure and integration time) from inhalation will be printed. Arrays, which will be stored on the logical unit 95, may also be printed on screen or line printer for one selected time step. This will be controlled by the variable NTIMD. The time course of concentration- and dose values may be printed for a special grid point, which have to be defined by IFACHS and IEINR2. Here the time course of the specific tritium concentrations will be printed from the first hour of the reemission phase till the hour NSTOP.

Additionally, collective doses will be calculated and printed on paper but they will not be stored on a permanent file.

Up to now there exists no evaluation program for the results calculated in UFOTRI. In the future, the evaluation programs COCDOS, CORPER and CORARE of the COSYMA package, might be modified for the output of UFOTRI.

8.4 Example of a job control data set

Table 5 shows an example of a job control file with all the parameters of the general input groups of UFOTRI which are necessary to run the program. The parameters which belong to the input group TRIDAT are only a selection of those parameters which can be chosen by the user. But for each run the user should take care which parameters have to be modified and which can remain unchanged.

For running the program the user needs 5 FORTRAN members namely **TEILO**, **TEIL1**, **TEIL4**, **SCOMMON** and **PARAM**. TEILO includes the data statements for the general and most of the optional namelists as well as the read statements and control output of the frame of UFOTRI. TEIL1 contains the main program. As mentioned at the beginning, the COMMON blocks used in the UFOTRI-frame are implemented in the SCOMMON part which will be imbedded by an INCLUDE statement in the single program parts. Due to some historical reasons the COMMON blocks in the dispersion part of UFOTRI are separated from those of the SCOMMON part. Nevertheless most of the COMMON blocks which are in SCOMMON occur in the dispersion part too. So be careful if you change one of the COMMON blocks. Some general dimension parameters are defined in PARAM which is imbedded in SCOMMON. TEIL4 contains the main subroutine with the name

UFOTRI calculating the dispersion-, ingestion- and dose part of the UFOTRI code. There exist two TEIL4 members, containing the different subroutines of the two IMSL-library versions.

All necessary and optional input/output units are listed in Table 4.

8.5 Examples of NAMELIST input

The programs of UFOTRI are written in standard FORTRAN-77 with the use of two additional features, the INCLUDE and NAMELIST statements.

The INCLUDE statement causes the FORTRAN compiler to insert lines taken from another file into the file being compiled. It is used to insert COMMON blocks into most of the subroutines of the UFOTRI programs. The statement takes the form

```
INCLUDE(filename)
```

in the source code provided. This may need to be modified for some computers. For example, the equivalent statement on a VAX computer is

```
INCLUDE 'file.FOR'/LIST
```

where file.FOR is the name which has been given to the file to be included as it was copied from the UFOTRI tape to the user's computer.

If the INCLUDE statement is not available on the user's computer, then the required lines must be inserted using an editor.

Within UFOTRI FORTRAN NAMELISTs are used to provide a free format input together with default values for all the parameters considered. The user-supplied input only needs to specify values for those parameters for which the default is not considered applicable. Full details of the way this is done will be given in the Fortran language manual for the computer system in use. This section gives a brief summary of the main features of NAMELIST input. The input routines will have to be extensively re-written if the package is to be used on computer systems without this feature.

The Fortran program contains statements like the following:

```
DIMENSION REALS(5),INTEG(5)
DATA REALS/1.0,2.0,3.0,4.0,5.0/
DATA INTEG/5,5,3,0,0/
DATA PARAM/10.0/
DATA INTPAR/0/

NAMELIST /EXAMPL/ REALS, INTEG, PARAM, INTPAR

READ(5,EXAMPL)
```

These statements define floating point (e.g. for storing decimal numbers) variables REALS and PARAM. REALS is an array of 5 members which have default values REALS(1)

= 1.0, REALS(2) = 2.0, REALS(3) = 3.0, REALS(4) = 4.0, and REALS(5) = 5.0 PARAM is a single variable and has the default value of 10.0. The statements also define integer variables INTEG and INTPAR. INTEG is also an array of 5 members which have default values INTEG(1) = 5, INTEG(2) = 5, INTEG(3) = 3, INTEG(4) = 0, and INTEG(5) = 0. INTPAR is a single variable with default value of 0.

All or any of these default values can be changed from the input file. The section of the file referring to these parameters is introduced by

```
&EXAMPL
```

Note that the & must be in the second column of the line on which it appears. The rest of the input section is written in free format, and terminated by &END.

Examples of the input file follow.

```
&EXAMPL
  INTEG(1) = 1,  INTEG(5) = 1
&END
```

This sets the values of INTEG(1) and INTEG(5) to be 1, and leaves all the other parameters, including the other members of the array INTEG, at their default values. Note that the variable names used in the input must be identical to those used in the program.

```
&EXAMPL
  REALS = 5*2.3
&END
```

This sets all five members of the array REALS to the value 2.3, and leaves all other parameters at their default values.

```
&EXAMPL
  PARAM=5.0,  INTPAR=3
&END
```

This sets only the variables PARAM and INTPAR, leaving the other variables at their default values.

```
&EXAMPL      &END
```

This leaves all variables at their default values. Note that this must be used to leave the variables at default values unless the NAMELIST is optional or keywords are used to input certain NAMELISTs only.

References

- /1/ Baldocchi, D.D., Hicks, B.B. and Camara, P.
A Canopy Stomatal Resistance Model for Gaseous Deposition to Vegetated Surfaces
Atmospheric Environment, Vol. 21, No. 1, pp. 91-101 (1987)
- /2/ Belot, Y., Gauthiers, D., Camus, H. and Caput, C.
Prediction of the Flux of Tritiated Water from Air to Plant Leaves.
Health Physics, Vol. 38, pp. 575-583 (1979)
- /3/ Brown, R.M., Ogram, G.L. and Spencer, F.S.
Field Studies of HT Oxidation and Dispersion in the Environment I. The 1986 August Experiment at Chalk River
Canadian Fusion Fuels Technology Project, G-88007 (1988)
- /4/ Brutsaert, W.H.
Evaporation into the Atmosphere
D. Reidel Publishing Company, Dordrecht, Holland (1982)
- /5/ Camillo, P. J. and Gurney, R.
A Resistance Parameter for Bare-Soil Evaporation Models
Soil Science, Vol. 141, No. 2, pp. 95-105 (1986)
- /6/ Currie, J. A.
Gaseous diffusion in porous media. Part 2.-Dry granular materials
British J. of App. Physics, Vol. 11, pp. 318-324 (1960)
- /7/ Diabate, S.
Personal communication, (1992)
- /8/ DLG
DLG-Futterwerttabellen: Mineralstoffgehalte in Futtermitteln,
Frankfurt, 1973
- /9/ Dunstall, T.G. and Ogram, G.L.
Diffusion and Biological Oxidation as Component Processes Regulating the Deposition of Tritiated Hydrogen to Soils
Ontario Hydro Research Division, Canada, Report Nr. 90-235-k (1990)

- /10/ Fisher, M.J. et. al.
An Analysis of the Effects of Repeated Short-term Soil Water Deficits on Stomatal Conductance to Carbon Dioxide and Leaf Photosynthesis by the Legume *Macroptilium atropurpureum* cv. Siratro
Australian Journal of Plant Physiology, Vol. 8, pp. 347-357 (1981)
- /11/ Garland, J.A.
The Absorption and Evaporation of Tritiated Water Vapor by Soil and Grassland Water, Air and Soil Pollution, Vol. 13, pp. 317-333 (1980)
- /12/ Geißler, G.
Pflanzenbau, 2. verb. Auflage,
Verlag Paul Parey, Berlin-Hamburg, (1988)
- /13/ Goudriaan, J.
A simple and fast numerical method for the computation of daily totals of crop photosynthesis,
Agricultural and Forest Meteorology, Vol. 38, pp. 249 - 254, (1986)
- /14/ Groh, A. und Steinhauer, C.
COMA: Programmbeschreibung
Interner Bericht, Kernforschungszentrum Karlsruhe (1987)
- /15/ Guenot, J. and Y. Belot
Assimilation of ^3H in Photosynthesizing Leaves Exposed to HTO
Health Physics Vol. 47, No.6, pp. 849-855 (1984)
- /16/ Hasemann, I. and Jones, J.A.
COSYMA: User Guide
CEC Brussels EUR-report 13045 (1991)
KfK-report 4331 B, Kernforschungszentrum Karlsruhe (1991)
- /17/ Jarvis, P.G.
The Interpretation of the Variation in Leaf Water Potential and Stomatal Conductance Found in Canopies in the Field
Phil. Trans. R. Soc. London, Vol. B 273, pp. 593-610 (1976)
- /18/ COSYMA: A New Program Package for Accident Consequence Assessment
A Joint Report of KfK and NRPB
Commission of the European Communities, Report EUR-13028 EN (1991)

- /19/ McIntosh, D.H., and Thom, A.S.
Essentials of Meteorology.
Wykeham Science Series 3, London (1969)
- /20/ Kim, J. and Verma, S. B.
Modelling the canopy photosynthesis: scaling up from a leaf to canopy in a temperate grassland ecosystem,
Agricultural and Forest Meteorology, Vol. 57, pp. 187 - 208, (1991)
- /21/ R. C. Mitchell et al.
Dark respiration of winter wheat crops in relation to temperature and simulated photosynthesis,
Annals of Botany, Vol. 67, pp. 7-16 (1991)
- /22/ V. Moses and M. Calvin
Photosynthesis Studies with Tritiated Water,
Biochim. biophysica Acta, Vol. 33, pp. 297-312 (1959)
- /23/ Penman, H.L.
Evaporation: An Introductory Survey
Netherl. J. Agric. Sci., Vol. 4, pp. 9-29 (1956)
- /24/ Raskob, W.
UFOTRI: Program for Assessing the Off-Site Consequences from Accidental Tritium Releases
KfK-report 4605, Kernforschungszentrum Karlsruhe, June 1990
- /25/ Raskob, W.
User Guide for UFOTRI: A Program for Assessing the Off-Site Consequences from Accidental Tritium Releases
KfK-report 4853, Kernforschungszentrum Karlsruhe, March 1991
- /26/ Raskob, W.
Modelling of the Tritium Behaviour in the Environment
in: Proceedings of the '4th Topical Meeting on Tritium Technology in Fission, Fusion, and Isotopic Applications' Albuquerque, 29.9.91 - 4.10.91,
Fusion Technology, 21, 2, pp. 636-645 (1992)

- /27/ Ritchie, J.T.
Model for Predicting Evaporation from a Row Crop with Incomplete Cover
Water Resources Research, Vol. 8, No.5, pp. 1204-1213 (1972)
- /28/ Rutter, A.J.
The Hydrological Cycle in Vegetation.
in: Monteith, J.L. (Ed.): Vegetation and the Atmosphere, Vol. 1, Academic Press
London (1975), pp. 111-154
- /29/ Shaw, P.V., Haywood, S.M.
A Dynamic Model for Predicting the Movement of Tritium in the Environment
Radiation Protection Dosimetry, Vol. 16, No.1-2, pp. 59-62 (1986)
- /30/ Schenk, R.
Zum Einfluß der Wasserversorgung, Mineraldünger und Bodenverdichtung auf die
Nährstoffaufnahme und den Ertragsbildungsverlauf bei Kartoffeln,
Dissertation, Humboldt-Universität Berlin, (1990)
- /31/ Seller, P.J.
Canopy reflectance, photosynthesis and transpiration,
International Journal of Remote Sensing, Vol. 6, No. 8, pp. 1335 - 1372, (1985)
- /32/ Shu Fen Sun
Moisture and Heat Transport in a Soil Layer Forced by Atmospheric Conditions.
M.Sc. thesis
University of Connecticut (1982)
- /33/ Spencer, F.S., and Dunstall, T.G.
Molecular Tritium Conversion in Vegetation, Litter and Soil.
Radiation Protection Dosimetry, Vol. 16, No. 1-2, pp. 89-93 (1986)
- /34/ Souci, S.W.
Die Zusammensetzung der Lebensmittel,
Nährwerttabellen 1981/82, Stuttgart, (1989)
- /35/ Statistisches Bundesamt / Wiesbaden
Statistisches Jahrbuch für die Bundesrepublik Deutschland (1988)
- /36/ Straka, J., Geiß, H. and Vogt, K.J.
Diffusion of Waste Air Puffs and Plumes under Changing Weather Conditions
Contr. Atm. Phys., Vol. 54, pp. 207 - 221 (1981)

- /37/ Turner, D.B.
Workbook of Atmospheric Dispersion Estimates. Public Health Service Publication
No. 999-AP-26 (1970)
- /38/ Walley, W.J., and Hussein, D.E.D.A
Development and Testing of a General Purpose Soil-Moisture-Plant Model
Hydrological Sciences Journal, Vol. 27, No. 1, pp. 1-17 (1982)
- /39/ Weir, A. H.
A winter wheat crop simulation model without water or nutriment limitations,
Journal of Agricultural Science, Camb., Vol. 102, pp. 371 - 382, (1984)

subroutine	description
EBALAF	balances a matrix
EHESFF	reduces the matrix to the upper Heisenberg form
EHBCKF	formes the matrix of accumulated transformations
EQRH3F	calculates the eigenvalues and eigenvectors
EBBCKF	transforms the eigenvectors to a balanced matrix to those of the original unsymmetric matrix
VSRTDR	orders the eigenvalues in descending order
LINV2F	calculates the inverse of the eigenvector matrix
VMULFF	multiplication of two matrices
LEQTIC	solve a complex general system of linear equations

Table 2. Old IMSL-subroutines called in the long term ingestion part (COMA)

subroutine	description
DEVCRG	computes all the eigenvectors and eigenvalues of a real matrix
DWRCRN	prints a complex rectangular matrix with integer row and column labels
DLFCRG	computes the LU factorization of a real general matrix and estimate its L1 condition number
DLFIRG	uses iterative refinement to improve the solution of a real general system of linear equations
DWRRRN	transforms the eigenvectors to a balanced matrix to those of the original unsymmetric matrix
DWRRRN	prints a real rectangular matrix with integer row and column labels
DMRRRR	multiplies two real rectangular matrices
DLFTCG	computes the LU factorization of a complex general matrix
DLFSCG	solves a complex general system of linear equations given the LU factorization of the coefficient matrix

Table 3. New IMSL-subroutines called in the long term ingestion part (COMA)

unit	output	input	definition
NEIN	----	INDAT	user NAMELIST input (default: 5)
NAUS	INDAT	----	printout of input data and results (default: 6)
11	----	UFOTRI	meteorological data in UFOTRI form; direct access file
13	(METSAM)	METEO	starting times and probability of the weather sequences (only if LWOPT = 2 and LPOPT = 2)
21	UFOTRI	----	results of UFOTRI
31	(GRIDS)	METEO	input file for the population data (if NSTOPT = 3)
91	UFOTRI	----	plot information for testing some parameters for special grid points
92	UFOTRI	----	plot information for testing some parameters (areas)
93	UFOTRI	----	plot information about time course of concentrations (point value)
95	UFOTRI	----	arrays with doses from inhalation and ingestion pathways with and without food restrictions

Table 4. Sorted list of I/O-Units for the tritium model UFOTRI

```

//INR303X1 JOB (0303,102,P0D5S),RASKOB,REGION = 6000K,NOTIFY = INR303,
// MSGCLASS = H,TIME = (0,30)
//*****
//*                               *
//* ---> TEST JCL                 *
//*                               *
//*****
/*MAIN LINES = 50
// EXEC F7CLG,PARM.C='INCLUDE',
//      IMSL = DP
//C.SYSPRINT DD DUMMY
//C.SYSINC DD DISP = SHR,DSN = INR303.UFOTRI.FORT
//C.SYSIN DD DSN = INR303.UFOTRI.FORT(TEIL0),DISP = SHR
//      DD DSN = INR303.UFOTRI.FORT(TEIL1),DISP = SHR
//      DD DSN = INR303.UFOTRI.FORT(TEIL4),DISP = SHR
//G.SYSIN DD *
@
@
@      FK2
@
POLGRID
&GRDPAR
IMAX = 20,JMAX = 72,
R = 65., 100., 145., 210., 320., 460., 680., 1000.,
1500.,2100., 3200., 4600., 6800., 10000., 15000., 21000., 32000.,
46000., 68000., 100000.,
RA = 80., 120., 170., 260., 390., 570., 840.,
1250., 1750., 2600., 3900., 5700., 8400., 12500., 17500., 26000.,
39000., 57000., 84000., 125000.
&END
ISOTOPE
&ISOPAR
NABL = 2,
VA = 5.E-4,0.005
&END
SOURCE
FKxy      1      0      0
          1      20 0.000E0 0.000E0 0.000E0
METEOZON
KARLSRHE      1      1 0 1 2 10
4020
00HOMOGEN      0 1.00E-0      1
5.00E+01      0

```

```

PRINTOUT
&OUTPAR
NOOTKZ = 2,NOOTMT = 2
&END
METEOROL
&METPAR
METIN = 0,IWNDR = 315,IWNDG = 300,IREGN = 100,IDIKAT = 4,
MIXLH = 1600,1200,800,560,320,200
&END
END
&TRIDAT
NJAHRE = 1,LWETE = 1,INUKL = 2,IPRPLT = 1,IWRITE = 0,
IDMP = 8,IDMPMX = 15,JDMP = 1,JDMPMX = 72,IFACHS = 13,
IEINR1 = 6,IEINR2 = 8,IEINR3 = 10,IEINR4 = 12,
NSTOP = 70,BODFAK = 10.,REMRE = 0.3,IZFREI = 3600,IFLENG = 0,BODEIN = 0.198,
IRFIX = 0,REFEST = 0.50,ITEMPE = 1500,ISTRBE = 500,ISTRGR = 200,
IZUSD = 0,IZUAUS = 0,KAUSDR = 1,1,1,0,0,0,0,0,0,0,0,
Q(2,1) = 1.,Q(1,1) = 0.0,Q1 = 3.7E14,
NBOX = 10,NINI = 10,NINT = 10,NOUT = 10,ITIMD = 9,NCOW = 250,
WWCOW = 350.,WOCOW = 150.
TIMEDO = 0.,3.,7.,14.,21.,30.,90.,180.,200.,365., 370., 3650.,
FAKC1 = 0.2,FAKC2 = 0.4,FAKCP = 0.2,FAKCW = 0.2,
RCMIN = 2.,LEAF = 3.,BEWG = 1440.,BEWGZ = 160,
RCMIN2 = 2.,LEAF2 = 3.,BEWG2 = 680.,BEWGZ2 = 170.,
RCMINP = 2.,LEAFP = 4.7,BEWGP = 2700.,BEWGZP = 300.,
RCMINW = 2.,LEAFW = 7.,BEGW = 2000.,BEWZW = 500.,
IPOT = 192,IWHEAT = 261,IMILK = 315,IVEGE = 165,IMEAT = 206,
DOSHT = 6.8E-16,DOSFOB = 4.0E-11,BRRATE = 2.67E-4,
IMODEL = 1,IARTBO = 1,WILTP = 0.1,SOILMX = 0.5,IBODEX = 1,
IMONT = 1,IRRIGA = 0,IRRIGG = 0,IFLAGS = 1,IFLAGR = 1,IDEPHT = 1,
IBODFX = 0,ICOVER = 1,IRELIN = 181,IPHOTO = 1
&END
//G.FT11F001 DD DISP = SHR,DSN = INR303.TRYKLIMR.DATA,LABEL = (,,IN)
//G.FT13F001 DD DISP = SHR,DSN = INR303.STRTTIME.DATA,LABEL = (,,IN)
//G.FT21F001 DD UNIT = SYSDA,DCB = DCB.VBS,SPACE = (TRK,500)
//G.FT31F001 DD dummy
/*
//G.FT91F001 DD DISP = SHR,DSN = INR303.BEISPIEL.TRITDA1,LABEL = (,,OUT)
//G.FT92F001 DD DISP = SHR,DSN = INR303.BEISPIEL.TRITDA2,LABEL = (,,OUT)
//G.FT93F001 DD DISP = SHR,DSN = INR303.BEISPIEL.TRITDA3,LABEL = (,,OUT)
//G.FT95F001 DD DISP = SHR,DSN = INR303.BEISPIEL.TRITDA4,LABEL = (,,OUT)
//G.FT99F001 DD DISP = SHR,DSN = INR303.BEISPIEL.TRITDA5,LABEL = (,,OUT)

```

Table 5. Example of an UFOTRI Job Control file (cont. on next page)

subroutine	description
INPUT	input namelist UFODAT
PUNKTE	specifies grid points
DOSREL	time dependent dose conversion factors
COVER	development stage of plants
AUSBPF	area source dispersion + short term ingestion
LIFTOF	Lift-off criteria and building wake
PLRISE-HOEHE	final rise
PQYZFO	vert. interpolation of diff. coefficients
PQYZF2	vert. interpolation of diff. coefficients (narrow)
DRYDEP-INTEG	dry deposition to soil
DRYPF	deposition to plants
HTDEP	deposition velocity HT
RISEFX	rising phase of the plume
OUTPA	control output
METOUT	controls output of met. data
ZEITNE	integration times with harvesting times
TRANSF	calculates transfer rates
COMA	long term ingestion pathway
INGES	dose calculations
DOSIS	collective dose calculation
OUTDAT	rearrangement of arrays for output
CNZOUT	printout and storage (optional)
PRIPLO	plot on screen
FOOBAN	food restriction calculation
FLAEB	area affected by food restrictions

Table 6. Subroutines called from UFOTRI (basis subroutine)

subroutine	description
BODENR	soil parameter + re-em. from soil
BODENR-RESIST	resistance of soil and plants
BODENR-MASSCH	mass balance check for plants
BODENR-WATER	extended soil transport module
DRYPF	deposition to plants
RESUS	re-emission rate from plants
FLAE	area source module (normal)
FLAE3	area source module (narrow)
PQYZFO	vertical interpolation of diff. coefficients
DRYDE2-INTEG	dry deposition to soil
TRANSF	calculates transfer rates

Table 7. Subroutines called in the area source module AUSBPF

subroutine	description
COMA	long term ingestion pathway
COMAS	first entry
COMA1	calculation of the transfer matrix
COMA1-EIGENS	all vector operations will be performed
COMA2	calculation of the actual and integral concentrations in all boxes
COMA2-CMACMP	analysis of imaginary solutions

Table 8. Subroutines called in the long term ingestion module COMA

transfer rate	from	to	value in d ⁻¹
$t_{1,1}$	atmosphere	outside	16.6
$t_{1,11}$	atmosphere	soil	0.68
$t_{1,14}$	atmosphere	plant HTO	0.325
$t_{11,1}$	soil ₁₁	atmosphere	0.20
$t_{11,12}$	soil ₁₁	soil ₁₂	0.21
$t_{11,14}$	soil ₁₁	plant HTO	$4.2 \cdot 10^{-2}$
$t_{12,11}$	soil ₁₂	soil ₁₁	$1.2 \cdot 10^{-2}$
$t_{12,13}$	soil ₁₂	soil ₁₃	$6.6 \cdot 10^{-2}$
$t_{12,14}$	soil ₁₂	plant HTO	$4.1 \cdot 10^{-2}$
$t_{13,12}$	soil ₁₃	soil ₁₂	$8.2 \cdot 10^{-3}$
$t_{13,13}$	soil ₁₃	ground water	$8.2 \cdot 10^{-3}$
$t_{13,14}$	soil ₁₃	plant HTO	$2.8 \cdot 10^{-2}$
$t_{14,1}$	plant HTO	atmosphere	3.6
$t_{14,15}$	plant HTO	plant OBT	$2.5 \cdot 10^{-3}$
$t_{15,14}$	plant OBT	plant HTO	$3.2 \cdot 10^{-2}$

Table 9. Transfer rates of the first COMA subsystem: agricultural area with leafy vegetables: (transfer rates calculated with standard input values)

transfer rate	from	to	value in d^{-1}
$t_{1,1}$	atmosphere	outside	16.6
$t_{1,2}$	atmosphere	<i>soil</i> ₁	0.68
$t_{1,5}$	atmosphere	grass HTO	0.32
$t_{1,7}$	atmosphere	cow HTO	$4.9 \cdot 10^{-5}$
$t_{2,1}$	<i>soil</i> ₁	atmosphere	0.20
$t_{2,3}$	<i>soil</i> ₁	<i>soil</i> ₂	0.17
$t_{2,5}$	<i>soil</i> ₁	grass HTO	$8.3 \cdot 10^{-2}$
$t_{3,2}$	<i>soil</i> ₂	<i>soil</i> ₁	$1.2 \cdot 10^{-2}$
$t_{3,4}$	<i>soil</i> ₂	<i>soil</i> ₃	$2.45 \cdot 10^{-2}$
$t_{3,5}$	<i>soil</i> ₂	grass HTO	$6.2 \cdot 10^{-2}$
$t_{4,3}$	<i>soil</i> ₃	<i>soil</i> ₂	$8.2 \cdot 10^{-3}$
$t_{4,4}$	<i>soil</i> ₃	outside	$8.2 \cdot 10^{-3}$
$t_{5,1}$	grass HTO	atmosphere	7.6
$t_{5,6}$	grass HTO	grass OBT	$8.1 \cdot 10^{-3}$
$t_{5,7}$	grass HTO	cow HTO	$2.2 \cdot 10^{-2}$
$t_{6,5}$	grass OBT	grass HTO	$2.4 \cdot 10^{-2}$
$t_{6,7}$	grass OBT	cow HTO	$1.8 \cdot 10^{-2}$
$t_{6,8}$	grass OBT	cow OBT	$2.9 \cdot 10^{-3}$
$t_{6,10}$	grass OBT	milk OBT	$1.5 \cdot 10^{-3}$
$t_{7,1}$	cow HTO	atmosphere	$3.0 \cdot 10^{-2}$
$t_{7,2}$	cow HTO	<i>soil</i> ₁	0.13
$t_{7,8}$	cow HTO	cow OBT	$1.1 \cdot 10^{-3}$
$t_{7,9}$	cow HTO	milk HTO	$3.9 \cdot 10^{-2}$
$t_{7,10}$	cow HTO	milk OBT	$1.3 \cdot 10^{-3}$
$t_{8,7}$	cow OBT	cow HTO	$1.5 \cdot 10^{-2}$
$t_{8,10}$	cow OBT	milk HTO	$2.1 \cdot 10^{-3}$

Table 10. Transfer rates of the second COMA subsystem: grass with meat/milk pathway: (transfer rates calculated with standard input values)

transfer rate	from	to	value in d^{-1}
$t_{p1,p1}$	atmosphere	outside	16.6
$t_{p1,p2}$	atmosphere	<i>soil</i> ₁	0.68
$t_{p1,p5}$	atmosphere	potato HTO	0.41
$t_{p2,p1}$	<i>soil</i> ₁	atmosphere	0.14
$t_{p2,p3}$	<i>soil</i> ₁	<i>soil</i> ₂	0.26
$t_{p2,p5}$	<i>soil</i> ₁	potato HTO	$4.2 \cdot 10^{-2}$
$t_{p2,p7}$	<i>soil</i> ₁	tuber HTO	$8.7 \cdot 10^{-3}$
$t_{p3,p2}$	<i>soil</i> ₂	<i>soil</i> ₁	$1.2 \cdot 10^{-2}$
$t_{p3,p4}$	<i>soil</i> ₂	<i>soil</i> ₃	$7.7 \cdot 10^{-2}$
$t_{p3,p5}$	<i>soil</i> ₂	potato HTO	$4.4 \cdot 10^{-2}$
$t_{p3,p7}$	<i>soil</i> ₂	tuber HTO	$8.8 \cdot 10^{-3}$
$t_{p4,p3}$	<i>soil</i> ₃	<i>soil</i> ₂	$8.2 \cdot 10^{-3}$
$t_{p4,p4}$	<i>soil</i> ₃	outside	$8.2 \cdot 10^{-3}$
$Tp45$	<i>soil</i> ₃	potato HTO	$2.9 \cdot 10^{-2}$
$t_{p4,p7}$	<i>soil</i> ₃	tuber HTO	$5.8 \cdot 10^{-3}$
$t_{p5,p1}$	potato HTO	atmosphere	2.4
$t_{p5,p6}$	potato HTO	potato OBT	$5.3 \cdot 10^{-3}$
$t_{p5,p7}$	potato HTO	tuber HTO	$2.0 \cdot 10^{-1}$
$t_{p5,p8}$	potato hto	tuber OBT	$2.6 \cdot 10^{-3}$
$t_{p6,p5}$	potato OBT	potato HTO	$6.9 \cdot 10^{-2}$
$t_{p7,p5}$	tuber HTO	potato HTO	$4.7 \cdot 10^{-1}$

Table 11. Transfer rates of the third COMA subsystem: potatoes: (transfer rates calculated with standard input values)

transfer rate	from	to	value in d^{-1}
$t_{p1,p1}$	atmosphere	outside	16.6
$t_{p1,p2}$	atmosphere	soil ₁	0.68
$t_{p1,p5}$	atmosphere	potato HTO	0.304
$t_{p2,p1}$	soil ₁	atmosphere	0.21
$t_{p2,p3}$	soil ₁	soil ₂	0.20
$t_{p2,p5}$	soil ₁	wheat HTO	$3.9 \cdot 10^{-2}$
$t_{p3,p2}$	soil ₂	soil ₁	$1.2 \cdot 10^{-2}$
$t_{p3,p4}$	soil ₂	soil ₃	$6.3 \cdot 10^{-2}$
$t_{p3,p5}$	soil ₂	wheat HTO	$3.9 \cdot 10^{-2}$
$t_{p4,p3}$	soil ₃	soil ₂	$8.2 \cdot 10^{-3}$
$t_{p4,p4}$	soil ₃	outside	$8.2 \cdot 10^{-3}$
$Tp45$	soil ₃	wheat HTO	$2.6 \cdot 10^{-2}$
$t_{p5,p1}$	wheat HTO	atmosphere	2.4
$t_{p5,p8}$	wheat HTO	wheat OBT	$1.2 \cdot 10^{-2}$
$t_{p5,p7}$	wheat HTO	seedling HTO	0.32
$t_{p5,p8}$	wheat HTO	seedling OBT	$4.1 \cdot 10^{-3}$
$t_{p8,p5}$	wheat OBT	wheat HTO	$6.9 \cdot 10^{-2}$
$t_{p7,p5}$	seedling HTO	wheat HTO	8.3

Table 12. Transfer rates of the fourth COMA subsystem: wheat: (transfer rates calculated with standard input values)

Figure 14. Basic flow-chart of UFOTRI: (Storage units for testing and countermeasures not included)

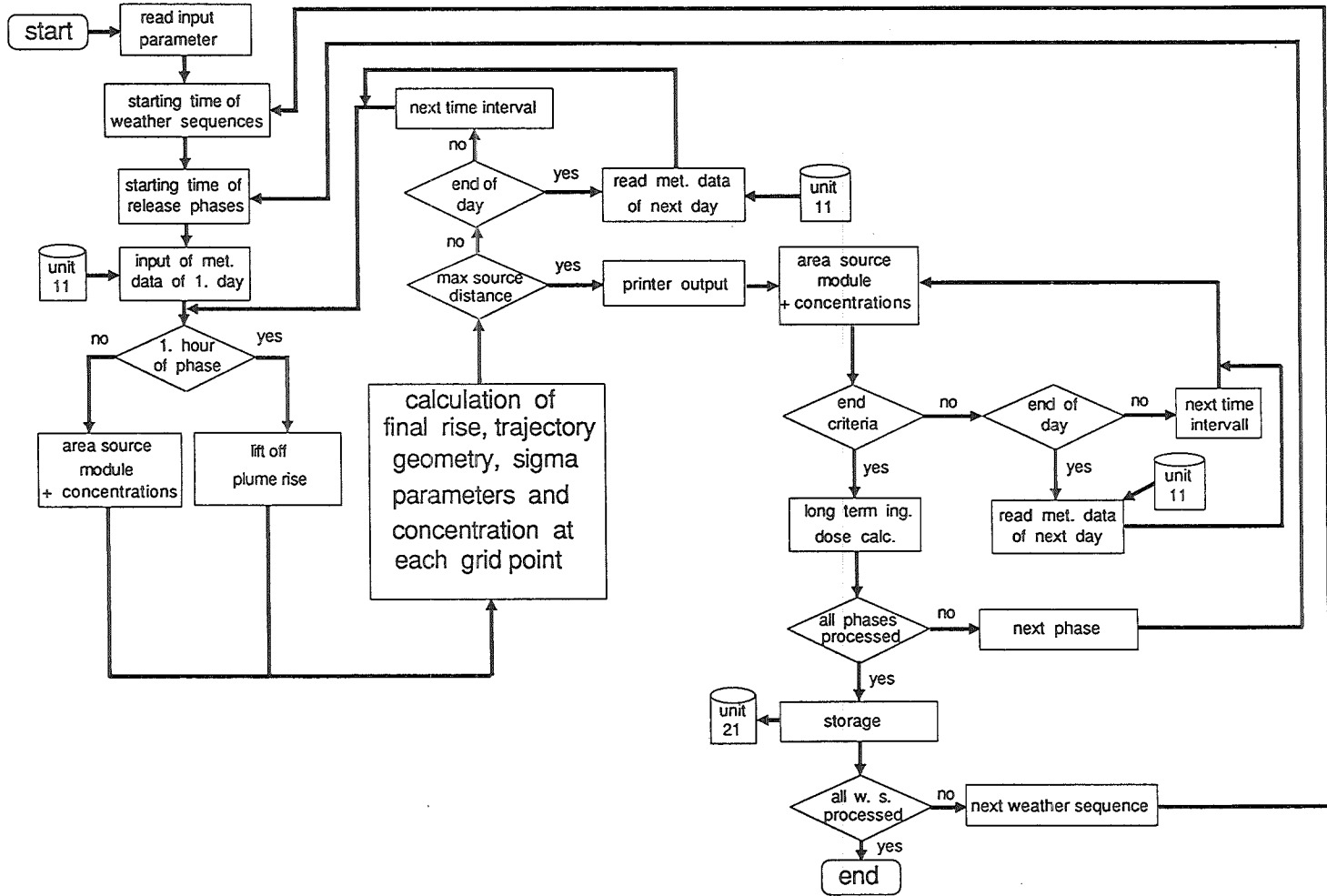


Figure 15. Flow-chart of area source dispersion module AUSBPF

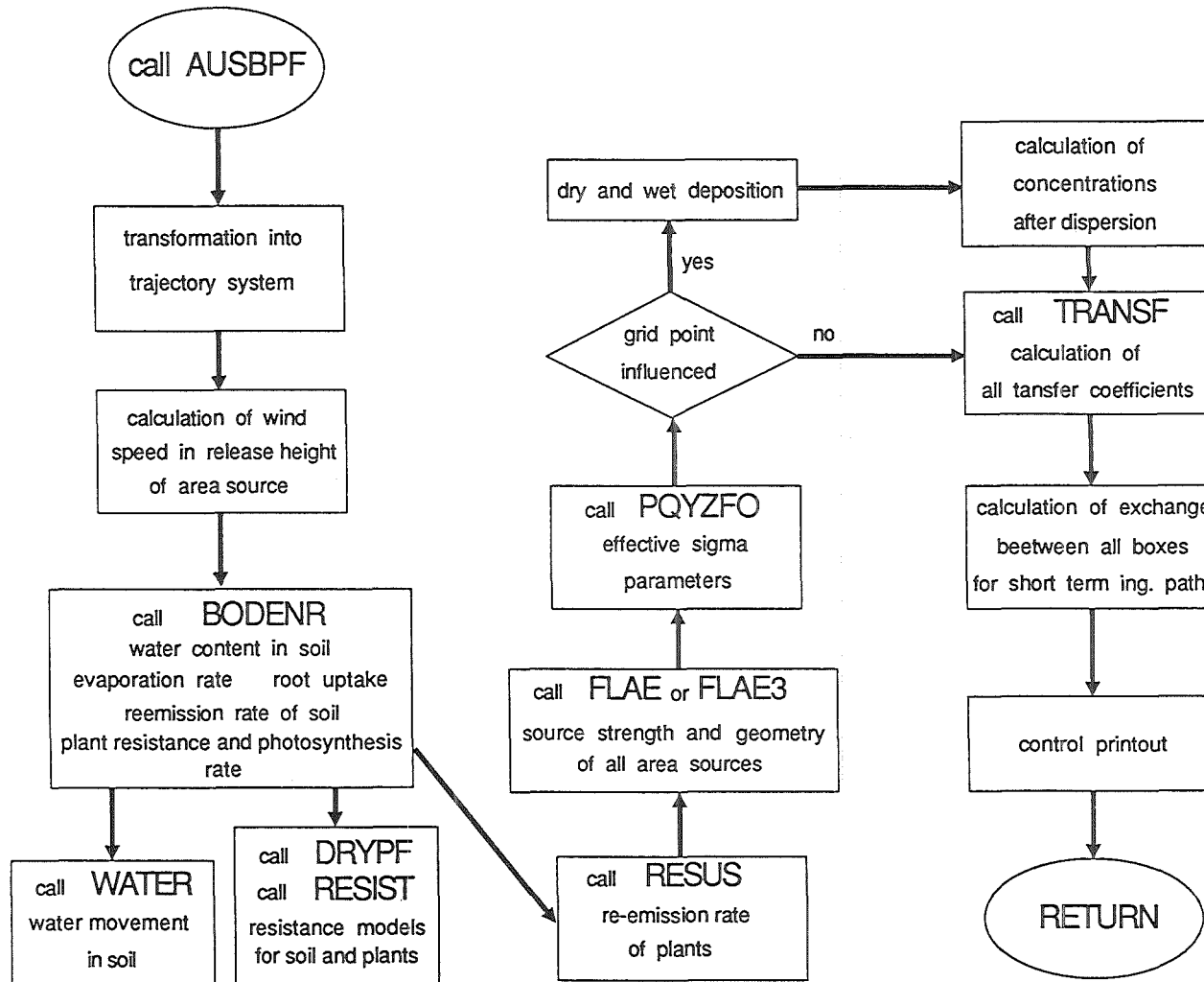


Figure 16. Flow-chart of long-term ingestion module COMA

